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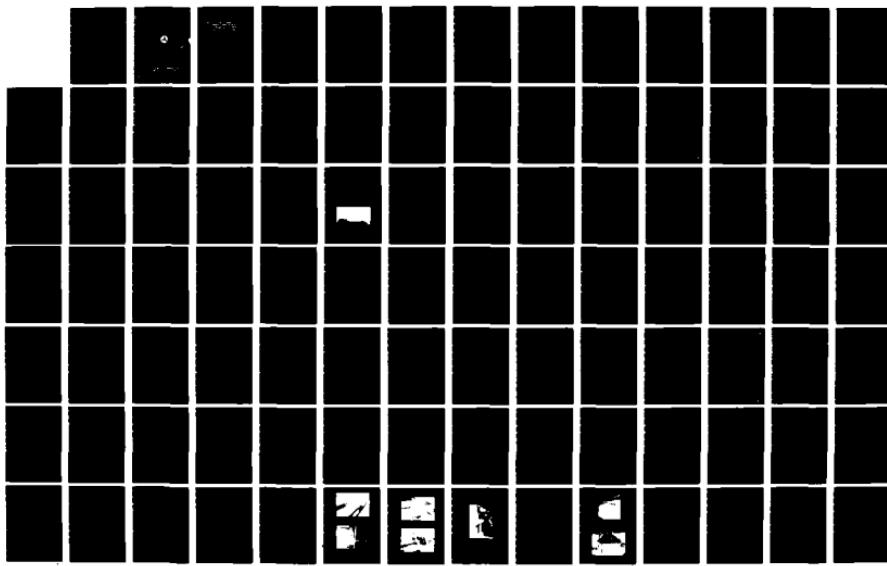
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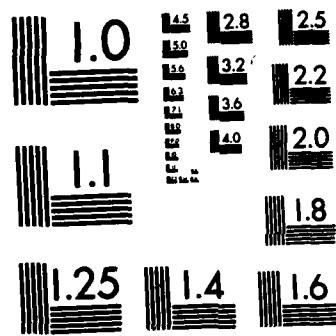
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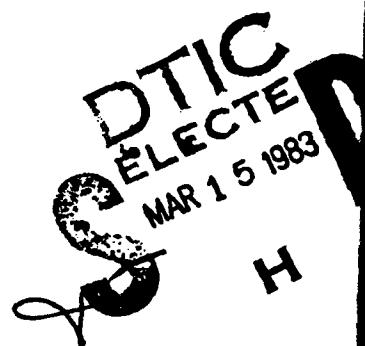
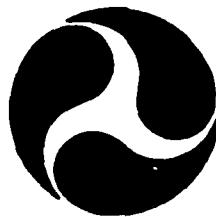


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ANALYTICAL AND EXPERIMENTAL STUDY TO IMPROVE
COMPUTER MODELS FOR MIXING AND DILUTION OF
SOLUBLE HAZARDOUS CHEMICALS

FRANKLIN T. DODGE
J. CHRISTOPHER BUCKINGHAM
THOMAS B. MORROW



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**ANALYTICAL AND EXPERIMENTAL STUDY
TO IMPROVE COMPUTER MODELS
FOR MIXING AND DILUTION OF
SOLUBLE HAZARDOUS CHEMICALS**

by
Franklin T. Dodge
J. Christopher Buckingham
Thomas B. Morrow

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16. Abstract	<p>Computerized models are developed to predict the concentration of soluble chemicals in various types of water bodies from accidental spills from, say, punctured ship tanks. Separate models are developed for continuous and instantaneous spills. Positively- and negatively-buoyant chemicals are considered, and the initial mixing and dilution due to gravitational and momentum effects are included. For downstream regions, turbulent mixing and dispersion are modeled as well. If the spill is in a tidal river, time-varying effects are included, as is the possibility that the water may pass by the spill site more than once.</p> <p>Predictions of the models are compared to the results of tests conducted in a large laboratory channel, with generally good agreement. The tests cover a wide range of chemical densities, spill rates, spill volumes, and channel water velocities. Extensive data on concentration distributions are reported.</p>		
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LIST OF SYMBOLS

Common Symbols

A	= transverse location of spill origin from river center.
B	= depth of spill origin below river surface.
C	= chemical concentration in river.
d	= depth of river.
e_x	= dispersion coefficient for a depth-mixed spill.
e_t	= time-varying part of e_x for a tidal river.
E_x	= dispersion coefficient for a cross-section-mixed spill.
E_t	= time-varying part of E_x for a tidal river.
g	= acceleration of gravity.
M_0	= initial mass of instantaneous spill.
M	= mass discharge rate of continuous spill.
n	= roughness factor for river surfaces.
r	= radial coordinate.
t	= time; $t = 0$ at spill initiation.
t_e	= time duration of a continuous spill.
T	= duration of tidal period.
u	= river velocity.
u_0	= steady part of tidal river velocity.
u_1	= amplitude of unsteady part of tidal river velocity.
u_s	= shear (friction) velocity.
w	= width of river.
w_s	= $A + w/2$.
x,y,z	= coordinate system (see Figure III.1).
y_n, z_n	= coordinates of n^{th} image (see Figure III.1).
α	= tidal phase at $t = 0$.
$\epsilon_x, \epsilon_y, \epsilon_z$	= turbulent diffusivities.
ρ	= water density.
ρ_c	= chemical density.

Symbols Used Only in Continuous Spill Models for a Steady River

b	= width of constant concentration region, Colenbrander's model.
b_o	= characteristic plume radius, Ooms' model.

LIST OF SYMBOLS (CONTD.)

c_*	= plume centerline concentration, Ooms' model.
c_A	= plume centerline concentration, Colenbrander's model.
C_d	= fluid drag coefficient on plume, Ooms' model.
E	= mass flowrate of chemical into plume, Colenbrander's model.
H_{eff}	= effective plume height, Colenbrander's model.
k	= von Karman's constant.
K	= proportionality constant, Eq. (III.17).
L	= length and width of chemical pool, Colenbrander's model.
Q_{max}	= E/L^2 .
R_n	= defined by Eq. (III.44b).
Ri_*	= Richardson number definition, Colenbrander's model.
s	= path length variable along plume centerline.
S_y, S_z	= cross channel and vertical dispersion coefficients.
u^*	= plume centerline velocity relative to current.
u'	= turbulence entrainment velocity, equal to u_* .
U	= plume velocity, Ooms' model.
U_o	= characteristic velocity for power-law profile.
W	= effective width of concentration profile, Colenbrander's model.
x_{NF}	= maximum downstream length for near-field model.
x_{OIF}	= maximum downstream length for intermediate-field model.
x_{OOMS}	= maximum downstream length for Ooms' model.
Δx_{IF}	= location of virtual origin, intermediate-field model.
Δx_{NF}	= location of virtual origin, near-field model.
y'	= cross-stream coordinate measured from plume centerline.
z_o	= characteristic depth in power-law velocity profile.
\bar{z}, z'	= z-coordinate measured upward from channel bottom if $\rho_c > \rho$ or from surface downward if $\rho_c < \rho$.
α	= exponent in power-law velocity profile.
$\alpha_1, \alpha_2, \alpha_3$	= entrainment coefficients, Ooms' model.
β	= exponent in experimental power-law correlation for point-source dispersion coefficient, equal to 0.5 for a river or channel.
γ	= mass decay coefficient (evaporation), Colenbrander's model.
$\Gamma()$	= gamma function.

LIST OF SYMBOLS (CONTD.)

δ	= proportionality constant in σ_y correlation.
θ	= plume angle from horizontal, Ooms' model.
λ	= ratio of effective concentration width to plume velocity width, Ooms' model.
ρ	= density of diluted chemical plume.
σ_y	= cross-channel dispersion coefficient for a point source.
ω_n	= defined by Eq. (III.46).

Symbols Used Only in Instantaneous Spill Models

d_0	= initial diameter of spill cloud.
h_c	= thickness of spill cloud, function of time.
h_0	= initial thickness of spill cloud.
M	= chemical mass in cloud, $M_0 - M_e$.
M_e	= chemical mass evaporated from cloud.
N	= number of point or line sources in near- and intermediate-field models.
N_{Ri}	= Richardson number definition in Eidsvik's model.
r_c	= radius of cloud, function of time.
t_{ONF}	= near-field time that gives peak concentration equal to that of the gravity-spreading model at $t = t_{VNF}$.
t_{VNF}	= maximum time for validity of gravity-spreading model.
Δt_{NF}	= virtual-time origin of near-field model.
u_{side}	= entrainment velocity around the sides of cloud.
u_{top}	= entrainment velocity over the top of the cloud.
θ	= defined by Eq. (III.70).
ρ_{mix}	= density of diluted chemical cloud.

Symbols Used Only in Continuous Spill Models for Tidal Rivers

C_j	= leading term in intermediate-field model, Eq. (III.78).
t_j	= time at which the water that is at the observation point at the observation time was previously at the spill origin $x = 0$.
u_j	= river velocity at time t_j .
\bar{u}_j	= average river velocity over time period $t - t_j$.

LIST OF SYMBOLS (CONTD.)

Symbols Used Only in Similitude Analysis

D = diameter of puncture.
Fr = densimetric Froude number of chemical spill = $\frac{\rho u^2}{(\rho_c - \rho) gd}$
J = ratio of initial plume momentum to river velocity = $\frac{\rho_c U^2}{\rho u^2}$
SC_x = sensitivity coefficient.
Vi = volume of instantaneous spill.
λ = scale factor.
ν = kinematic viscosity of river water.
θ_c = angle from horizontal of initial plume.

Symbols Used Only in Appendix A

τ = time at which point (or line) instantaneous source is injected into water.
ξ = integration variable.

Symbols Used Only in Appendix B

\bar{C} = time and cross-section averaged concentration.
 C_0, C_1, \dots = approximation functions of total concentration.
 $\bar{u}, \bar{u}_0, \bar{u}_1$ = time and cross-section averaged river velocity, and steady and tidal amplitudes.
 m_e = evaporated mass per unit surface area.
 ζ = $x - \int u dt$ = transformed space variable.
 τ = transformed time variable.
 ϕ_1 = correction to C_1 approximation.

Symbols Used Only in Appendix C

$\bar{\delta}$ = effective half-length of each instantaneous point (or line) source at the observation point at the observation time.

I. EXECUTIVE SUMMARY

This final report covers all four tasks of a project to revise and verify experimentally the mixing and dilution models for water soluble chemicals of the Hazard Assessment Computer System (HACS). The report documents (1) the analysis, development, and verification of the final form of the models, (2) all experimental procedures and representative test data, and (3) listings of the computerized models suitable for HACS.

Background

Analytical/computer models had been developed previously for the U. S. Coast Guard for use in predicting the mixing and dilution of water-soluble chemicals spilled into waterways. A later independent review found that the models contained a number of serious limitations and errors:

1. Only neutrally-buoyant spills are considered.
2. The initial momentum and size of the spill are neglected.
3. The evaporation model is uncoupled from the mixing and dilution models.
4. Discontinuous concentrations are predicted where the "near field" and "far field" dilution models are matched.
5. The time-dependency of the flow in tidal rivers is neglected.
6. Coastal waters and estuaries are not included.

For those reasons, the Coast Guard has sponsored the present program to correct the indicated deficiencies and to validate the revised models experimentally.

Task 1 - Literature Review and Reformulation/Revision of Models

After reviewing the literature on spills in water and the analogous case of plumes in air, it was determined that major revisions were needed to the models to predict the chemical concentrations in the "near field" close to the spill; the methods used by the existing HACS models do not represent the best available state-of-the-art techniques and generally give unreliable

predictions in the area where the concentrations are the highest and the hazards the greatest. For regions farther downstream, the form of the existing models was satisfactory although errors in some of the empirical correlation equations and in the "near field" - "far-field" matching had to be eliminated.

In summary, three new models were developed:

1. Continuous spill in a steady river;
2. Instantaneous spill in a steady or tidal river; and
3. Continuous spill in a tidal river.

For estuaries and coastal waters, an existing "Dynamic Estuary Model" was examined and recommended for use but further development of that model was not attempted during this program.

In addition to turbulent diffusion and dispersion of the chemical discharge downstream of the spill, the model of a continuous spill now includes (1) the effects of the momentum and buoyancy of the chemical stream discharged from a punctured tank on the dilution of the resulting plume, and (2) the buoyancy-induced spreading and dilution of the plume where it impacts the channel bottom or water surface. Those parts of the model are partially based on well-verified models of the dispersal of a heavy gas discharged in the air or along the ground. In addition, the model accounts for the effects of the channel boundaries on the concentration and includes evaporation from a plume that reaches the water surface.

The model of an instantaneous spill includes buoyancy-induced spreading and dilution near the spill site, as well as turbulent diffusion and dispersion farther downstream. The effects of the channel boundaries and evaporation are also treated. The analysis is partially based on analogous models of a heavy-gas cloud spreading along the ground. For a tidal river, the effects of the transient tidal flow on the mixing and dilution are included, as derived from an original analysis.

The model for a continuous spill in a tidal river is similar to that for a steady river, with one major exception. Analytical difficulties in treating buoyancy-induced mixing in a transient flow made it impractical to include such mixing in the model. Thus, the predictions are likely to be less accurate for negatively- or positively-buoyant chemical spills in the near-field than the corresponding steady-river model. The effects of the tidal flow are included, however, as is the possibility that water can pass back-and-forth by the spill site several times.

The models now can be used for nearly every practical combination of chemical density, spill duration, spill rate, spill volume, and waterway type. They have been programmed for computerized solution, and program listings and flow charts are given in this report.

Task 2 - Experimental Design

In order to verify the model predictions, an extensive test program was designed. Because of a lack of suitable test facilities for the simulation of a tidal flow, the test program considered only steadily-flowing rivers. Moreover, the emphasis was on verification of the model predictions for regions near the spill site, since for areas farther downstream the models are similar to well-understood and well-developed diffusion and dispersion models. A sensitivity analysis of the models was conducted to aid in the test design; this analysis revealed the parameters that have the most influence on the concentration predictions and therefore should require control and accurate measurement. The test plan was approved by the Coast Guard.

Task 3 - Data Collection and Analysis

Most of the tests covered in the Test Plan were conducted in a rectangular channel at Texas A&M University. The channel width of 1.52m and depth of 0.24 m was assumed to represent a scale reduction of 1 to 50 in order to select realistically-scaled values of the other test parameters.

After a number of preliminary tests and a subsequent revision of the test plan, a total of ten instantaneous spills and nine continuous spills were

conducted. The tests covered a range of chemical specific gravities from 0.79 to 1.40, two river speeds for each chemical, and either two spilling rates or two spilled volumes (depending on the type of spill) for each chemical.

The chemicals were mixed with measured quantities of a fluorescent dye so that concentrations could be determined by a fluorometer, using small samples taken from the channel. For most of the tests, concentrations were measured, at one or more downstream locations, over the channel width and depth, as well as with respect to time for instantaneous spills.

Task 4 - Revision and Demonstration of the Mathematical Models

In this task, the models of continuous and instantaneous spills in a steady river were compared to the test data, and the "best" values of certain empirical constants appearing in the models were selected. For each kind of spill, the results of several of the tests were used to make the selection of the empirical constants. The remaining tests were then used as independent data for model verification. Generally good comparisons of the models and the test results were obtained.

It is concluded that the revised models are now satisfactory for use in the Hazard Assessment Computer System.

II. INTRODUCTION

As part of the Hazard Assessment Computer System of the Chemical Hazards Response Information System, models have been developed to predict the mixing, dilution, and evaporation of water soluble chemicals spilled into waterways from accidental punctures of cargo ship tanks [1, Models 4 and 11]. Since the models are to be used primarily for contingency planning and the evaluation of responses to accidents in progress, their formulation was general enough to treat a variety of waterways, spill sizes, and spill durations without the need to describe water velocity profiles, bottom roughnesses, waterway cross-sections, puncture shapes, and other characteristics of the accident that are unlikely to be available in practice. They were, therefore, more idealized than a corresponding model developed specifically for a given spill and waterway would need to be. A critical review [2] has shown that, even so, the models are overly limited in scope and contain errors in their basic physical representations. For those reasons, the Coast Guard has sponsored the present program to correct the indicated deficiencies and to validate the revised models experimentally.

The previous review [2] and the review conducted as part of the present work have concluded that the primary criticisms and limitations of the available models are:

1. Only neutrally-buoyant spills are considered.
2. The initial momentum and size of the spill are neglected.
3. The evaporation model is uncoupled from the mixing and dilution models.
4. Discontinuous concentrations are predicted where the "near field" and "far field" dilution models are matched.
5. The time-dependency of the flow in tidal rivers is neglected.
6. Coastal waters and estuaries are not included.

The first two comments imply that the models will not adequately represent many types of spills. For a continuous spill, for example, the buoyancy of the chemical as it enters the water has a strong effect on the initial mixing,

as would its initial momentum [3]. Further, if the initial buoyancy (negative or positive) is not dissipated by the time the plume intersects the waterway bottom or free surface, the chemical will be mixed by gravity across the waterway width more rapidly than would be predicted by the mixing and dilution analyses incorporated in the available models [4]. As a result of the deficiency cited in the third comment, more chemical can be evaporated than was contained in the original spill while, at the same time, the originally spilled mass is still predicted to be contained in the waterway. To correct the deficiency given in the fourth comment, a proper accounting of the spilled mass or mass flow rate must be used in matching the various model regimes. There are two limitations implied by the fifth comment. First, the differences between the diffusion and dispersion coefficients of a tidal river and a steadily-flowing river are not predicted correctly [5]. Second, the possibility that water can flow back-and-forth under the spill site several times is neglected. (A tidal river is here defined to be that upstream part of an estuary where density, i.e., salinity, gradients are negligible but where the flow velocity oscillates with the tides.) The sixth comment implies that the models are limited to waterways with a defined and uniform flow direction. Other criticisms can be made of the correlating equations used to compute diffusion and dispersion coefficients and of certain other details of the models, but those listed above cite the major deficiencies.

The present program was designed to reformulate the models in the light of the above criticisms and to validate the models experimentally. The program efforts were arranged into four tasks.

Task 1 - Literature Review and Reformulation/Revision of Models

For this task, the mixing-dilution-evaporation models for water soluble chemicals were reformulated to remove the limitations and correct the deficiencies listed above.

Task 2 - Experimental Design

For this task, a set of experiments was designed to validate the reformulated models, with emphasis on near-field mixing and dilution where

the initial momentum and buoyancy of the spill are important.

Task 3 - Data Collection and Analysis

For this task, the experimental program designed in Task 2 was executed. The experiments were conducted in a large water channel at Texas A&M University.

Task 4 - Revision and Demonstration of Mathematical Models

For this task, the reformulated models were compared to the experimental results and revised as indicated by the comparisons. Each model was also computerized and documented.

This report is generally organized in agreement with the four tasks; the major exception is that the model revisions indicated by the test results are incorporated in the descriptions of the models at the time they are first given. All the data from the tests are presented in the companion Test Data Volume of this Final Report.

III. REFORMULATION OF MODELS

III.1 Common Assumptions and Remarks

The models developed in this report are based upon a small number of common assumptions, which have been made primarily to eliminate the need for a detailed description of the waterway and the spill rather than to simplify the basic physical representations. To avoid repetition, the assumptions are listed together here.

Waterway Assumptions

W.1 - The waterway is straight and has a constant width, w , and depth, d . The effect of the waterway dimensional configuration is characterized by the value of the hydraulic radius, R_h .

W.2 - The turbulent nature of the river or channel flow is characterized by the value of the friction velocity, u_* [5].

W.3 - The flow is assumed to be one-dimensional and the direct effects of the vertical and horizontal velocity profiles are neglected with two exceptions:

- (1) The vertical velocity profile is used in the near-field model for a continuous spill to compute the plume trajectory and rate of vertical dispersion.
- (2) The flow is assumed to be locally two-dimensional in the estuary model.

W.4 - The blockage and interference effects due to the presence of the cargo ship in the waterway are neglected.

Spill Assumptions

S.1 - A continuous spill is characterized by a constant mass flow rate, the density of the chemical, a specified spilling duration, and the diameter of a circular puncture.

S.2 - An instantaneous spill is characterized by the total mass of chemical released and the chemical density.

S.3 - The spilled chemical is infinitely soluble in water, and has the same temperature as the water.

Evaporation Assumption

E.1 - Evaporation is considered only for buoyant chemicals in which the concentration is high in the near-field regime at the waterway surface.

The consequences of these assumptions, many of which are commonly made in mixing and dilution studies, are not severe. The waterway assumptions together imply that localized effects, due to bends in the waterway, large scale roughness elements, and so on, cannot be predicted, nor can gradual increases or decreases of the mixing and dilution due to gradual changes in the cross-section area. The spill assumptions are all reasonable; the computerized form of the models in fact point out when an instantaneous spill is so large that it should be considered as continuous. Most of the chemicals of interest to the Coast Guard, and to which these models are meant to apply, are so highly soluble that Assumption S.3 is completely satisfactory. The evaporation assumption is a consequence of the high solubility of the chemicals; the partial vapor pressures of the dissolved chemicals are so low that evaporation is negligible unless the chemical "floats" at the surface with a high concentration.

The analytical models used to predict chemical concentrations from continuous and instantaneous spills are presented in Sections III.2 through III.5. Table III.1 summarizes the presentations and can serve as a guide for reference. In general, the models for any specific type of waterway would be used sequentially in the listed order to follow the fate of the spill.

Initially, it was proposed to allow the models to accept experimental data, say in the well-mixed region, for the purpose of improving the prediction accuracy of the models in the near-field regions. These kinds of composite analytical/experimental models did not prove to be feasible in terms of the accuracy required for the data-sample location with respect to the plume (or cloud) centerline. They will not be discussed further in this report.

III.2 Continuous Spills in Steady Rivers

In this section a navigable, non-tidal river is defined to be a flowing body of water of sufficient width and depth to permit the passage of loaded tank ships and barges. In the case of a rupture and complete discharge of a cargo tank, the amount of cargo released, M_0 , into the river may be known precisely. However, it is usually the rate of cargo release, M , that determines the peak concentrations downriver from the accident site. The cargo release rate depends upon the dimensions of the tank puncture and the hydrostatic pressure difference between cargo and water that causes the tank to drain. The HACS venting rate model has been revised and validated [6,7], and it may be used to estimate the cargo release rate from data furnished by field

TABLE III.1 GUIDE TO ANALYTICAL MODEL DEVELOPMENT

RIVER TYPE	SPILL TYPE	PHYSICAL APPLICATION	NAME	REPORT PAGES
Steady or Tidal	Continuous	Initial dilution of a buoyant plume, with significant momentum, before the plume impacts the river surface or bottom.	Ooms (very near-field)	13-17
Steady	Continuous	Dilution of a buoyant plume after it impacts the river surface or bottom.	Colenbrander (very near-field)	17-23
Steady	Continuous	Turbulent diffusion of a buoyant plume, after its buoyancy and momentum are negligible, that does not impact the river surface or bottom; or a plume without initial buoyancy or momentum.	Near-field	23-24
Steady	Continuous	Turbulent diffusion and dispersion of a plume well-mixed over the river depth.	Intermediate-field	24
Steady	Continuous, after discharge stops	Turbulent diffusion and dispersion of a finite-length plume	--	28-31
Steady or Tidal	Instantaneous	Initial dilution of a buoyant spill (cloud)	Eidsvik (very near-field)	32-38
Steady or Tidal	Instantaneous	Turbulent diffusion of a non-buoyant cloud	Near-field	39
Steady or Tidal	Instantaneous	Turbulent diffusion and dispersion of a cloud well-mixed over the river depth.	Intermediate-field	40-41
Steady or Tidal	Instantaneous	Turbulent dispersion of a cloud well-mixed over the river cross-section.	Far-field	41
Tidal	Continuous	Turbulent diffusion of a non-buoyant plume	Near-field	44-46
Tidal	Continuous	Turbulent diffusion and dispersion of a plume well-mixed over the river depth.	Intermediate-field	46
Tidal	Continuous	Turbulent dispersion of a plume well-mixed over the river cross-section.	Far-field	47
Tidal	Continuous, after discharge stops	Turbulent diffusion and dispersion of a finite-length plume	--	47-48
Bays & Estuaries	Continuous or Instantaneous	Dilution and dispersion of a non-buoyant spill in a water body that does not have a well-defined or predominant channel.	Dynamic Estuary Model	48-51

personnel at the accident site. Alternatively, the average release rate may be estimated as the amount of cargo released divided by the observed duration of the release. Discharges of short duration, say less than 10 minutes, should be analyzed as an instantaneous release. Discharges of more than 10 minutes duration will be analyzed by the continuous spill model.

III.2.1 General Description

The revisions that have been made to the mixing and dilution model for continuous spills in a steady river consist of

- o modeling the effects of the momentum and buoyancy of the discharged chemical on the trajectory and dilution (entrainment of water) of the chemical plume;
- o modeling the gravitational cross-stream spreading of the chemical plume after it reaches either the upper or lower surface of the river;
- o modeling the effect of density stratification between the chemical plume and the water on the rate of vertical entrainment;
- o improving the image modeling of the waterway boundaries; and
- o allowing for the simultaneous evaporation of chemical vapor from the surface of the chemical and water mixture.

The revised mixing and dilution model has three distinct phases of development. These are referred to as the

Very Near Field (VNF) - This phase occurs in a region close to the discharge point. Plume discharge momentum and buoyancy forces control the plume trajectory and influence the rates of vertical and horizontal spreading of the plume in this phase.

Near Field (NF) - This phase comprises the region in which momentum and buoyancy forces have a negligible effect on plume trajectory. Shear and turbulence generated by the river flow control the mixing and dilution of the chemical plume.

Far Field (FF) - This phase occurs when the chemical plume has been mixed uniformly over both the depth and width of the river. This phase occurs in a region that is far downriver from the spill site, and it may not be attained in rivers that are very wide.

In all three phases, evaporation of chemical vapor may occur from the river surface.

III.2.2 Very Near Field - Jet Momentum and Buoyancy Regime

In the region close to the discharge point, the discharged chemical stream is treated as a bent-over plume or jet. The rise and dispersion of buoyant gaseous plumes in air has received considerable attention in the air pollution literature [8]. Several models are available for predicting the plume rise and dilution of bent-over plumes in air [9]. The basic plume rise and dispersion processes are the same in water as in air. Therefore, one of the more general plume rise and dispersion models was selected for use in the very near field.

Ooms [3] developed a numerical (computer) model for bent-over plume development that solves four simultaneous differential equations for the conservation of mass, chemical species, and vertical and horizontal momentum. This model uses three empirical entrainment coefficients to quantify the entrainment of ambient fluid by velocity shear, buoyancy, and flow field turbulence. This model (unlike some of the algebraic plume rise formulas described in [9]) can be applied to plumes of positive, negative or neutral buoyancy with discharge angles between vertical and horizontal (downstream).

Ooms' model consists of a set of integral-differential equations that represent balances for chemical species, mass and momentum in a turbulent flowing ambient stream. The equations are

Conservation of chemical species

$$\frac{d}{ds} \left(\int_0^{b\sqrt{2}} 2\pi r C_U dr \right) = 0 \quad (\text{III.1})$$

Conservation of mass

$$\frac{d}{ds} \left(\int_0^{b\sqrt{2}} 2\pi r \bar{\rho} U dr \right) = 2\pi b \rho \{ \alpha_1 |u^*(s)| + \alpha_2 u |\sin \theta| \times \cos \theta + \alpha_3 u' \} \quad (III.2)$$

Conservation of momentum in the horizontal direction

$$\frac{d}{ds} \left(\int_0^{b\sqrt{2}} 2\pi r \bar{\rho} U^2 \cos \theta dr \right) = 2\pi b \rho u \{ \alpha_1 |u^*(s)| + \alpha_2 u |\sin \theta| \cos \theta + \alpha_3 u' \} + C_d \pi b \rho u^2 \sin^3 \theta \quad (III.3)$$

Conservation of momentum in the vertical direction

$$\frac{d}{ds} \left(\int_0^{b\sqrt{2}} 2\pi r \bar{\rho} U^2 \sin \theta dr \right) = \int_0^{b\sqrt{2}} g(\rho - \bar{\rho}) 2\pi r dr + C_d \pi b \rho u^2 \sin^2 \theta \cos \theta \quad (III.4)$$

The integrals in Equations (III.1) through (III.4) may be evaluated by assuming similarity profiles for the distribution of velocity, density and concentration in the plume

$$U(s, r, \theta) = u \cos \theta + u^*(s) e^{-r^2/b_0^2(s)} \quad (III.5)$$

$$\bar{\rho}(s, r, \theta) = \rho + \rho^*(s) e^{-r^2/\lambda^2 b_0^2(s)} \quad (III.6)$$

$$C(s, r, \theta) = c^*(s) e^{-r^2/\lambda^2 b_0^2(s)} \quad (III.7)$$

The plume density and concentration are related for isothermal flow as

$$\bar{\rho} = \frac{(\rho_c - \rho) C}{\rho_c} + \rho \quad (III.8)$$

where ρ_c is the density of undiluted chemical and ρ is the density of water.

The dependent variables in Equations (III.1) through (III.4) are the plume velocity u^* (not to be confused with u_* , the value of shear velocity for the river), the plume characteristic radius b_o , the angle of the plume with respect to horizontal θ , and the concentration c^* . The river velocity u is allowed to vary in the vertical direction as

$$u = U_o \left(\frac{\tilde{z}}{z_o} \right)^{\bar{\alpha}} \quad (III.9)$$

where

$$\tilde{z} = d - z \quad (III.10)$$

when z is directed vertically downward from the surface of the river as shown in Figure III.1. The parameters U_o , z_o , and $\bar{\alpha}$ are, ideally, determined from data fits to the velocity profile of the river under consideration. In the comparisons of model to test data described in Section V, U_o has been taken as the velocity at the surface, z_o has been taken as the river depth, and $\bar{\alpha}$ has been computed (using an analysis included in the computerized model) by reference to an assumed logarithmic profile based on the shear velocity; such a procedure would also be acceptable in actual applications with little loss of accuracy.

The differential equations that result from Equations (III.1) through (III.8) are integrated along the plume pathline s . Two additional differential equations are used to determine the plume trajectory

$$\tilde{z} = \tilde{z}_i + \int_0^s \sin \theta \, ds \quad (III.11)$$

$$x = x_i + \int_0^s \cos \theta \, ds \quad (III.12)$$

and x_i , \tilde{z}_i represent the coordinates of the discharge location.

Recommended values for the empirical model coefficients α_1 , α_2 , α_3 , C_d and λ^2 are given in Ooms' paper and are also discussed in [10]. The turbulence entrainment velocity u' will be equated to the turbulent shear velocity u_* in this study.

A computer program was written in FORTRAN to perform the numerical integration of Ooms' model equations. The effects of the river boundaries are simulated by means of a set of four first order images as

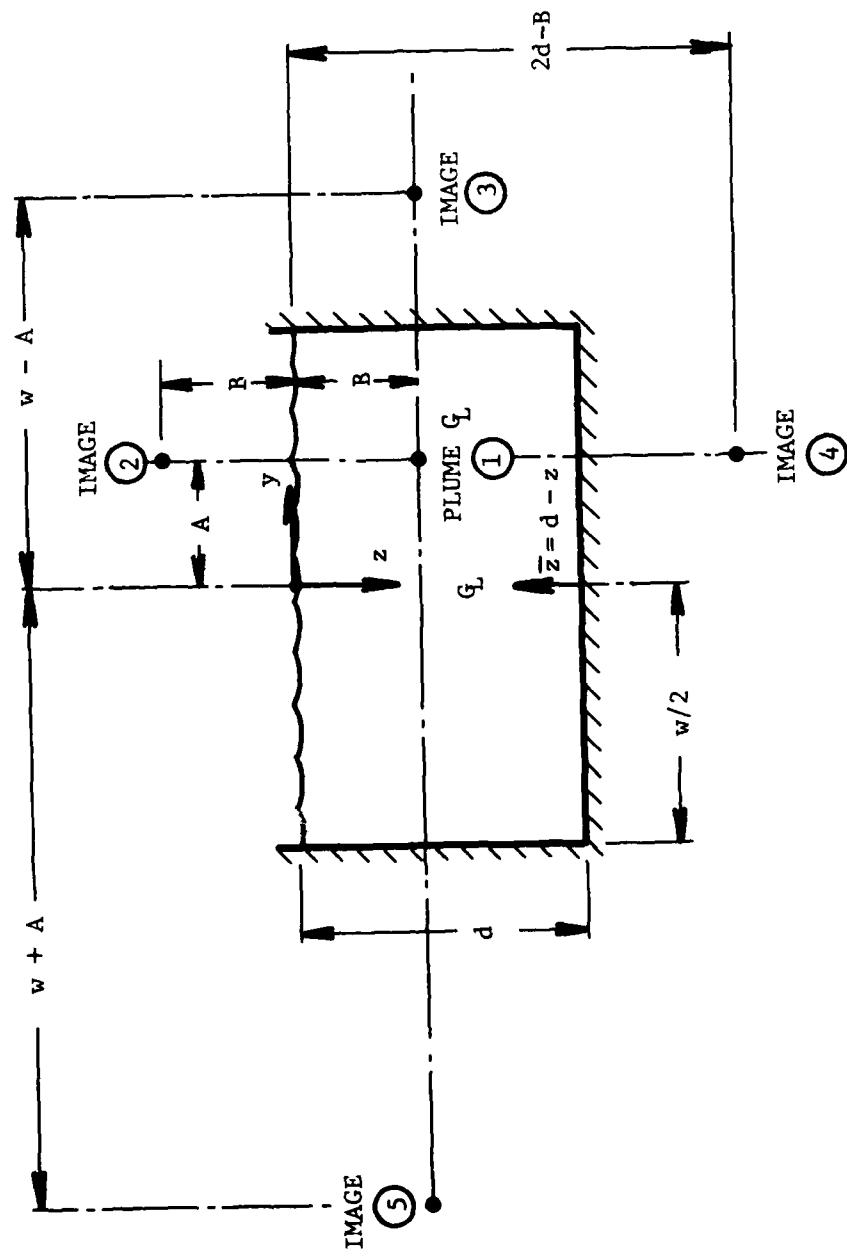


FIGURE III.1 COORDINATE SYSTEM FOR PLUME CENTERLINE AND FOUR FIRST-ORDER IMAGES

shown in Figure III.1. The concentration at a location x, y, z downriver from the discharge location can be expressed as

$$C(x, y, z) = c^* \sum_{n=1}^5 \exp \left[\frac{-(y-y_n)^2 - (z-z_n)^2}{\lambda^2 b_o^2} \right] \quad (\text{III.13})$$

For the arrangement shown in Figure III.1, the images are located at:

$y_1 = A, z_1 = B,$	plume centerline
$y_2 = A, z_2 = -B,$	image about the river surface
$y_3 = w-A, z_3 = B,$	image about the right bank
$y_4 = A, z_4 = 2d-B,$	image about the river bottom
$y_5 = (w+A), z_5 = B,$	image about the left bank

Plume development is continued with Ooms' model equations until a convenient point is reached for transition to another model. The transition criteria are

- o if the plume hits either the upper or lower river surface, transition to a second VNF model that includes buoyancy effects on lateral and vertical spreading for plumes developing over horizontal surfaces;
- o if the plume is very dilute (so that buoyancy effects are negligible), transition to a point source NF model;
- o if the plume dimensions are large with respect to the depth and/or width of the river, transition to a point source NF model.

III.2.3 Gravity Spreading Regime

Ooms' model can account for the effect of a nearby surface on the concentration field, but it cannot simulate the effect of the surface on the

plume trajectory. Therefore, if the chemical plume either rises to the river surface or sinks to the bottom, another model is required to continue the computation of plume development. Several models have been developed for the analogous atmospheric problem of the dispersion of a dense gas cloud close to the ground. We have selected Colenbrander's model [4] for the development of dense vapor clouds and adapted it to model the steady state behavior of a buoyant chemical plume above or below a river surface.

The laboratory tests reported in Sections IV and V show that when the value of Froude number associated with the chemical discharge is very low (about 0.5) the plume spreads out horizontally to form a pool when a surface is encountered. (The Froude number, which is effectively a ratio of the channel flow momentum to the buoyancy force exerted on the plume, is one of the parameters that controls the initial trajectory and dilution of the plume; see Section IV.1.3.) This behavior is shown in Figure III.2 for a discharge of sodium silicate at a Froude number of 0.51. As the flow of chemical (diluted by the entrainment of water) into the pool continues, the pool grows in size. However, the flow of water over the top of the pool entrains some of the chemical solution and transports it downriver. The rate of chemical uptake is influenced by the river speed, the shear velocity and the level of the density stratification characterized by the value of the



FIGURE III.2 FORMATION OF A POOL OF DENSE CHEMICAL SOLUTION OVER THE WATER CHANNEL FLOOR. SODIUM SILICATE, s.g. = 1.4, FROUDE NUMBER = 0.51

Richardson number. The plume that develops above the dense chemical pool is relatively broad in the cross-stream direction and thin in the vertical direction.

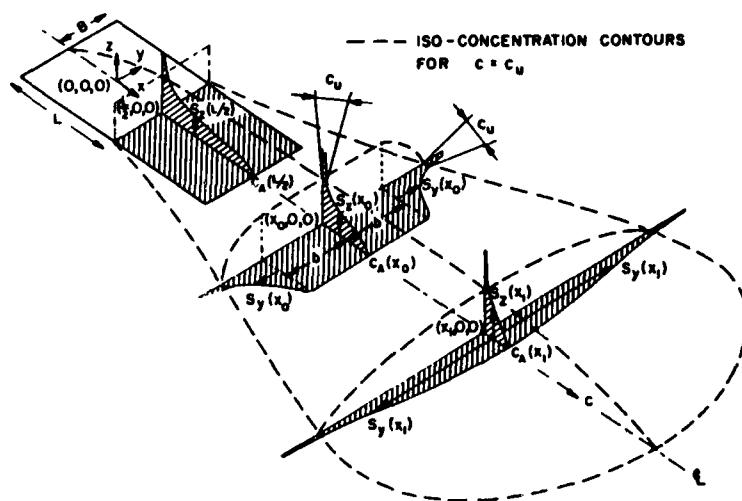
Colenbrander's model can be applied to this situation. It assumes that a dense fluid is taken up into the surroundings from a rectangular source area as shown in Figure III.3. Downwind from the area source the concentration distribution is approximated by similarity profiles

$$C(s, y, z) = C_A \exp \left[- \left(\frac{|y'| - b}{S_y} \right)^2 - \left(\frac{z'}{S_z} \right)^{1+\bar{\alpha}} \right] \quad (III.14)$$

for $|y'| > b$, and

$$C(x, y, z) = C_A \exp \left[- \left(\frac{z'}{S_z} \right)^{1+\alpha} \right] \quad (III.15)$$

for $|y'| < b$



THE SIMILARITY PROFILES FOR THE CONCENTRATION AND ISO-CONCENTRATION CONTOURS IN THE PLANES $y=0$, $z=0$, $x=x_0$, AND $x=x_1$

FIGURE III.3

Here, b is the width of a region near the plume centerline over which the concentration profile is independent of y' (the cross-stream distance measured from the plume centerline), and z' is a vertical dimension. For chemicals that are densre than water

$$z' = \tilde{z} = d - z$$

but for plumes of chemicals that are lighter than water

$$z' = z$$

The profile variables in Equations (III.14) and (III.15) are

- C_A , the plume centerline concentration
- b , the width of the constant concentration region
- S_y , the cross-stream dispersion coefficient, and
- S_z the vertical dispersion coefficient.

Colenbrander presents a set of differential equations that may be solved simultaneously to give the values of the profile variables as a function of the downstream distance.

The effective halfwidth (measured from $y' = 0$) of the plume is defined as

$$B_{eff} = b + \frac{\sqrt{\pi}}{2} S_y \quad (III.16)$$

Gravity spreading due to buoyancy causes the plume halfwidth to increase with distance as

$$\frac{d B_{eff}}{dx} = K \left[1 - \frac{\rho}{\bar{\rho}} \right]^{\frac{1}{2}} \left(\frac{S_z}{z_0} \right)^{\frac{1}{2} - \bar{\alpha}} \quad (III.17)$$

where

$$K = 1.0 \left(\frac{g z_0}{U_0^2} \right)^{\frac{1}{2}} \left[\Gamma \left(\frac{1}{1+\bar{\alpha}} \right) \right]^{\frac{1}{2}} (1+\bar{\alpha})^{-\frac{1}{2}} \quad (III.18)$$

The cross-stream dispersion coefficient increases with downstream distance due to the turbulent structure of the river flow. Thus

$$S_y \frac{d S_y}{dx} = \frac{4\beta}{\pi} W^2 \left[\frac{\delta \sqrt{\pi/2}}{W} \right]^{1/\beta} \quad (\text{III.19})$$

where

$$W = b + \frac{\sqrt{\pi}}{2} S_y \quad (\text{III.20})$$

and $\sigma_y = \delta x^\beta$ is a power law correlation for the cross-stream dispersion coefficient for a point source.

Equations (III.17) and (III.19) serve to determine the behavior of B_{eff} and S_y . The local value of b is calculated from Equation (III.16).

The vertical dispersion coefficient, S_z is determined from

$$\frac{d}{dx} \left[B_{eff} \left(\frac{S_z}{z_o} \right)^{1+\bar{\alpha}} \right] = \frac{k}{z_o} \frac{u_*}{U_o} (1+\bar{\alpha})^2 \frac{B_{eff}}{\phi(Ri_*)} \quad (\text{III.21})$$

where

k = the von Karman constant,

and $\frac{u}{U_o} = \left(\frac{z}{z_o} \right)^{\bar{\alpha}}$

is the assumed similarity form for the velocity profile, equivalent to Equation (III.9) above. The function $\phi(Ri_*)$ is an empirical correlation that models the effect of density stratification within the chemical plume on the vertical dispersion coefficient. Colenbrander suggests

$$\phi(Ri_*) = 0.74 + 0.25 Ri_*^{0.7} + 1.2 * 10^{-7} Ri_*^3 \quad (\text{III.22})$$

where Ri_* is the Richardson number defined as

$$Ri_* = g \frac{(\Delta\rho)}{\rho} \frac{H_{\text{eff}}}{u_*^2} \quad (\text{III.23})$$

and

$$H_{\text{eff}} = \Gamma \left(\frac{1}{1+\bar{\alpha}} \right) S_z / (1+\bar{\alpha}) \quad (\text{III.24})$$

is the effective height of the plume

The final equation for plume centerline concentration is

$$C_A = \frac{E(1+\bar{\alpha}) z_o^{\bar{\alpha}}}{U_o S_z^{1+\bar{\alpha}} B_{\text{eff}}} \quad (\text{III.25})$$

where E = mass flowrate of chemical taken up from the source into the plume. If desired, Equation (III.25) can be modified to include atmospheric evaporation of chemical from a buoyant plume that is spreading and developing along the river surface. If we assume that the concentration decreases at a rate that is proportional to the local concentration, then

$$C_A = \frac{E(1+\bar{\alpha}) z_o^{\bar{\alpha}}}{U_o S_z^{1+\bar{\alpha}} B_{\text{eff}}} e^{-\gamma x/u} \quad (\text{III.26})$$

A computer program was written in FORTRAN to perform the numerical integration of Colenbrander's model equations. As with Ooms' model, the effects of the river boundaries are simulated by a set of first order images.

The computation of plume development is continued with Colenbrander's model until the vertical dispersion coefficient is equal in

size to the river depth. At this point a transition is performed to the intermediate field line source model which assumes that the concentration field is well mixed in the vertical direction.

III.2.4 Turbulent Diffusion-Dispersion Regime

After the momentum-buoyancy-gravity phase of mixing is completed, a transition is made to a "near-field" model in which turbulent diffusion is the only important mixing mechanism. If buoyancy effects are not significant, a transition will take place directly from Ooms' model to a point source, near-field model.

When the point source model is used, the concentration is predicted from the solution to the standard turbulent diffusion equation [5]:

$$C(x,y,z) = \frac{\dot{M}}{4\pi x(\epsilon_y \epsilon_z)^{1/2}} \sum_{n=1}^5 \exp \left[-\frac{u(y-y_n)^2}{4x\epsilon_y} - \frac{u(z-z_n)^2}{4x\epsilon_z} \right] \quad (\text{III.27})$$

Here, y_n are the locations of the equivalent point source and its four first-order images. The images, as shown in Figure III.1, account for the dominant effects of the channel walls, bottom, and free surface; that is, they insure that $\partial C / \partial \bar{n} \approx 0$ at all those surfaces, where \bar{n} is the normal to the surface.

The turbulent diffusivities in Equation (III.27) are computed from the values of shear velocity and river depth:

$$\epsilon_z = 0.067 du_* \quad (\text{III.28})$$

and

$$\epsilon_y = K_\epsilon du_* \quad (\text{III.29})$$

Here, K_ϵ is 0.15 for a laboratory channel and is 0.6 for a river. The numerical constant of the ϵ_z correlation is recommended in [5], and the values of K_ϵ of the ϵ_y correlation have been chosen as a "best fit" to the extensive sets of data for rivers and channels given in [5].

The shear velocity is given as [11]

$$u_* = 3.807 n u / R_h^{1/6} \quad (III.30)$$

where $n \approx 0.009 \text{ (m)}^{1/6}$ for a "smooth" channel and $n \approx 0.025 \text{ (m)}^{1/6}$ for a river. The hydraulic radius is:

$$R_h = wd / (2d + w) \quad (III.31)$$

In Equation (III.27), the origin $x=0$ of the equivalent point spill is selected to match the very near-field concentration by a procedure discussed in Section III.2.5.

After the chemical plume has traveled some distance downstream the concentration distribution will become approximately uniform in the vertical direction. Plumes of negligible buoyancy that are modeled well by the point source Equation (III.27) become well mixed over the river depth at a distance of about $0.3ud^2/\epsilon_z$. Buoyant plumes with strong density stratification as modeled by Colenbrander's equations may require a longer distance before the vertical dispersion coefficient S_z becomes as large as the river depth, d . In either case, when the concentration distribution becomes nearly uniform in the vertical direction, a transition is made to a vertical line-source model that includes dispersion. The formulation suggested in [12] is used for this model since the effects of the channel surfaces are included exactly:

$$C(x,y) = \frac{\dot{M}}{wdu} \left[1 + 2 \sum_{m=1}^{\infty} \cos\left(\frac{m\pi w_s}{w}\right) \cos\left[\frac{m\pi(y+w/2)}{w}\right] \exp\left(-\frac{m^2\pi^2\epsilon_y x}{uw^2}\right) \right] \quad (III.32)$$

Here, the lateral dispersion coefficient ϵ_y is equal to ϵ_y for a constant-depth river [12], and w_s is the sum of A and $w/2$.

The origin $x=0$ of the line source is selected by a procedure discussed in Section III.2.5. Note that Equation (III.32) automatically reduces to the far-field concentration, \dot{M}/wdu , at locations far downstream.

III.2.5 Matching of Models

We shall first consider the matching conditions for plumes with strong buoyancy that either rise to the river surface or fall to the river bottom. The plume development is computed using Ooms' model until the plume centerline comes within a distance of $0.01 d$ of the upper or lower surface. When this occurs, a transition is made to Colenbrander's model and a set of matching conditions is applied to generate the initial values for model variables.

The laboratory experiments indicated that two types of transition were possible. For values of the densimetric Froude number of 0.6 and below, the chemical plume formed a pool on the surface. Chemical solution was taken up from the pool by turbulent entrainment into the flowing stream of water above or below the pool. However, for significantly higher values of Froude number, a pool was not formed. Instead, on reaching the surface, the plume would slump and spread laterally as it continued to move in a downstream direction. Both types of transition are considered here, with a test on the value of Froude number to determine which set is used.

For a value of Froude number less than 0.6, pool spreading is assumed. The amount of dilute chemical solution entering the pool is determined from the chemical discharge rate and the plume concentration:

$$\text{Mass flow into the pool} = \dot{M} [(\rho_c - \rho)/\rho_c + \rho/c_A] \quad (\text{III.33})$$

This number is equated to the rate of chemical solution uptake from the pool. The uptake rate is computed as

$$L^2 Q_{\max}^* = \frac{L \bar{\rho} z_0 U_0}{(1+\bar{\alpha})} \left(\frac{S_z}{z_0} \right)^{1+\bar{\alpha}} \quad (\text{III.34})$$

Since S_z is a function of distance, it is necessary to compute the uptake rate with the aid of a model equation for S_z

$$\frac{d}{dx} \left(\frac{S_z}{z_0} \right)^{1+\bar{\alpha}} = \frac{k}{z_0} \frac{u_*}{U_0} \frac{(1+\bar{\alpha})^2}{\phi(Ri_*)} \quad (\text{III.35})$$

At each x step, Equation (III.34) is evaluated (with $L = x$) and compared to the value of mass flowrate from Equation (III.33). When the two values of flowrate are equal, integration is stopped and the result used to determine initial values of S_z and $B_{eff} = L/2$. Also, we set $S_y = 0$ so that $b = B_{eff} = L/2$. The initial value of concentration is assumed to be equal to $2c^*$ where $2c^*$ is the value of the plume centerline concentration computed by Ooms' model with a first order image to give the effect of the river surface.

For values of Froude number greater than 0.6, the possibility of pool formation is neglected. Instead, the plume is assumed to flow along the river surface with initial values for the profile variables determined from the final values of plume variables computed by Ooms' model. As for the pool spreading case, we set

$$C_A = 2c^*$$

$$S_y = 0$$

Initial values of B_{eff} and S_z can be determined by integrating the profile formulas in the horizontal and vertical directions. First,

$$\int_0^{B_{eff}} C_A dy' = \int_0^{\infty} 2c^* e^{-(y'^2/\lambda^2 b_o^2)} dy' \quad (III.36)$$

gives

$$B_{eff} = \frac{\sqrt{\pi}}{2} \lambda b_o \quad (III.37)$$

Next,

$$C_A \int_0^{\infty} e^{-(z/S_z)^{1+\bar{\alpha}}} dz = \int_0^{\infty} 2c^* e^{-(z^2/\lambda^2 b_o^2)} dz \quad (III.38)$$

which gives

$$S_z = \frac{\sqrt{\pi}}{2} \lambda b_o / \Gamma\left(\frac{1}{1+\bar{\alpha}}\right) \quad (III.39)$$

For all other cases where the initial buoyancy of the plume is dissipated before the plume impacts the bottom or the free surface, the point source model is matched directly to the concentration predicted at the end of the valid range of Ooms' model. The end of Ooms' model is taken as the plume radius for which the concentration is $1/e$ of the starting value, since at that point the plume has lost most of its excess buoyancy and momentum. The corresponding plume radius is:

$$r_p = 0.50617 d/\lambda \quad (\text{III.40})$$

By referring to the equations of Ooms' model presented in Equations (III.1) to (III.12) and to Equation (III.27) of the point source model, it can be concluded that the origin of the point source model must be located at a distance upstream from the matching point equal to:

$$x_{ONF} = \lambda^2 r_p^2 u / 4\sqrt{\epsilon_y \epsilon_z} \quad (\text{III.41})$$

Letting x_{OOMS} represent the downstream distance from the spill at which Equation (III.40) occurs, the downstream offset from the actual spill site at which the virtual origin of the point source lies is:

$$\Delta x_{NF} = x_{OOMS} - x_{ONF} \quad (\text{III.42})$$

That is, at a given observation point, x , the value that must be used in the near-field model is $x - \Delta x_{NF}$. This matching procedure ensures (1) continuity of peak concentration, and (2) conservation of spilled mass; the concentration distribution of the two models may, however, be slightly different.

To match the intermediate-field line-source model to the near-field point source or Colenbrander model, the average concentration over the depth of the near-field model is computed at the downstream end of its range of validity; the average is made at the cross-stream location containing the peak concentration. A distance x in Equation (III.32) of Section III.2.4 is then determined (by an iterative procedure in the computerized models) such that the concentration predicted by the line-source model is equal to the

depth-averaged near-field concentration. Letting this distance be x_{OIF} , the virtual origin of the line source is thus shifted downstream from the actual spill site by an amount

$$\Delta x_{IF} = \Delta x_{NF} + x_{NF} - x_{OIF} \quad (III.43)$$

Here, x_{NF} is the downstream length for which the near-field model is valid, measured relative to its virtual origin. For a given observation point x , the value that must be used in the intermediate-field model is $x - \Delta x_{IF}$.

III.2.6 Concentrations After Discharge Ceases

After the discharge of chemical ceases at time t_e , the entire body of dilute chemical solution translates downstream with the river velocity. The concentration distribution is now affected by longitudinal dispersion as well as lateral and vertical diffusion and dispersion. However, if the observing location is positioned within the regimes modeled by either of the two VNF models (Ooms' or Colenbrander's model) the effect of longitudinal dispersion will be neglected. The local concentration will maintain its steady state value for an additional length of time equal to the upstream distance to the spill site divided by the river velocity. After that time, the concentration is assumed to be zero.

When the observing location is positioned within the near-field, point-source model regime, the concentration in the near-field can be computed by imagining that the discharge is made up of a stream of elementary discharges $dM = \dot{M}dt$ spread out in time over the period $t=0$ to $t=t_e$. The total effect is calculated by integration [5]. (When $t_e \rightarrow \infty$ or when the observation time t is less than t_e , this procedure gives the result obtained previously as Equation (III.27) of Section III.2.4.) Integration details are presented in Appendix A. The result is:

$$\begin{aligned}
C(x, y, z, t) = & \frac{\dot{M} \exp(ux/2 \epsilon_x)}{8\pi (\epsilon_y \epsilon_z)^{\frac{1}{2}}} \sum_{n=1}^5 \frac{1}{R_n} \left\{ \exp(uR_n/2\epsilon_x) \times \right. \\
& \left\{ \operatorname{erf} \left[\frac{R_n + u(t-t_e)}{\sqrt{4\epsilon_x(t-t_e)}} \right] - \operatorname{erf} \left[\frac{R_n + ut}{\sqrt{4\epsilon_x t}} \right] \right\} \\
& + \exp(-uR_n/2\epsilon_x) \left\{ \operatorname{erf} \left[\frac{R_n - u(t-t_e)}{\sqrt{4\epsilon_x(t-t_e)}} \right] - \right. \\
& \left. \operatorname{erf} \left[\frac{R_n - ut}{\sqrt{4\epsilon_x t}} \right] \right\} \quad (III.44a)
\end{aligned}$$

where

$$R_n = \left[x^2 + \frac{\epsilon_x}{\epsilon_y} (y - y_n)^2 + \frac{\epsilon_x}{\epsilon_z} (z - z_n)^2 \right]^{\frac{1}{2}} \quad (III.44b)$$

The longitudinal diffusion coefficient, ϵ_x , is difficult to estimate but is of the order of ϵ_y [5]. From our tests, as described in Section V.2, it appears that $\epsilon_x = 10 \epsilon_y$ is a realistic value.

Likewise, the intermediate field model is:

$$\begin{aligned}
C(x, y, t) = & \frac{\dot{M} \exp(ux/2 \epsilon_x)}{2w du} \left\{ \exp(ux/2\epsilon_x) \left\{ \operatorname{erf} \left[\frac{x + ut}{\sqrt{4\epsilon_x t}} \right] \right. \right. \\
& \left. \left. - \operatorname{erf} \left[\frac{x + u(t-t_e)}{\sqrt{4\epsilon_x(t-t_e)}} \right] \right\} + \exp(-ux/2\epsilon_x) \left\{ \operatorname{erf} \left[\frac{ut - x}{\sqrt{4\epsilon_x t}} \right] \right. \\
& \left. \left. - \operatorname{erf} \left[\frac{u(t-t_e) - x}{\sqrt{4\epsilon_x(t-t_e)}} \right] \right\} + 2 \cdot \sum_{n=1}^{\infty} \frac{\cos \frac{m\pi w_s}{w} \cos \frac{m\pi(y + w/2)}{w}}{\sqrt{4\epsilon_x \omega_m^2/u^2}} \times \right. \\
& \left. \dots \text{cont'd...} \right.
\end{aligned}$$

$$\begin{aligned}
& \left(\exp \left[x(u^2 + 4 e_x \omega_m^2)^{1/2} / 2 e_x \right] \left\{ \operatorname{erf} \left[\frac{t(u^2 + 4 e_x \omega_m^2)^{1/2} + x}{\sqrt{4 e_x t}} \right] \right. \right. \\
& \quad \left. \left. - \operatorname{erf} \left[\frac{(t-t_e)(u^2 + 4 e_x \omega_m^2)^{1/2} + x}{\sqrt{4 e_x (t-t_e)}} \right] \right\} \right. \\
& \quad \left. + \exp \left[-x(u^2 + 4 e_x \omega_m^2)^{1/2} / 2 e_x \right] \left\{ \operatorname{erf} \left[\frac{t(u^2 + 4 e_x \omega_m^2)^{1/2} - x}{\sqrt{4 e_x t}} \right] \right. \right. \\
& \quad \left. \left. - \operatorname{erf} \left[\frac{(t-t_e)(u^2 + 4 e_x \omega_m^2)^{1/2} - x}{\sqrt{4 e_x (t-t_e)}} \right] \right\} \right) \right) \quad (III.45)
\end{aligned}$$

where

$$\omega_m^2 = m^2 \pi^2 e_y / w^2 \quad (III.46)$$

The longitudinal dispersion coefficient is [12]

$$e_x = 5.93 du_* \quad (III.47)$$

After the spill ceases, the intermediate field model does not automatically reduce to the correct far-field limit. The longitudinal dispersion of a chemical mixed uniformly over the width and the depth is much greater than that for just uniform mixing over the depth [5]. By integrating a sequence of elementary discharges, the correct far-field model is found to be

$$\begin{aligned}
C(x, t) = & \frac{\dot{M} \exp(ux/2 E_x)}{2 wdu} \left\{ \exp(ux/2 E_x) \left\{ \operatorname{erf} \left[\frac{ut + x}{\sqrt{4 E_x t}} \right] \right. \right. \\
& \quad \left. \left. - \operatorname{erf} \left[\frac{u(t-t_e) + x}{\sqrt{4 E_x (t-t_e)}} \right] \right\} \right. \\
& \quad \left. + \exp(-ux/2 E_x) \left\{ \operatorname{erf} \left[\frac{ut - x}{\sqrt{4 E_x t}} \right] \right. \right. \\
& \quad \left. \left. - \operatorname{erf} \left[\frac{u(t-t_e) - x}{\sqrt{4 E_x (t-t_e)}} \right] \right\} \right) \quad (III.48)
\end{aligned}$$

The far-field longitudinal dispersion, as recommended by the data analysis of [13], is

$$E_x = 0.18 (u u_*)^{1/2} w^2 / R_h \quad (\text{III.49})$$

In use, the near-field model is assumed to be valid for a translated distance from the spill site equal to x_{NF} , as discussed in Section III.2.5; that is, Equation (44) is used for observation times and distances such that

$$0 \leq (x - \Delta x_{NF}) - u (t - t_e) \leq x_{NF} \quad (\text{III.50})$$

That part of the translating plume initially in the very near-field is also computed from the near-field model; this approximation will tend to overestimate the concentration.

The intermediate-field model, Equation (III.45) is assumed to be valid for observation times and distances such that

$$x_{NF} \leq (x - \Delta x_{IF}) - u (t - t_e) \leq u w^2 / e_y \quad (\text{III.51})$$

Likewise, the far-field model is used when

$$(x - \Delta x_{IF}) - u (t - t_e) > u w^2 / e_y \quad (\text{III.52})$$

These choices of matching points insure that the peak concentrations of the two matching fields are equal at the matching distance for $t = t_e$. But for $t > t_e$, the peak concentrations at the matching distances will no longer be equal, because the forward longitudinal dispersion rate of the upstream model will not be equal to the rearward longitudinal dispersion rate of the downstream model. This gradually-increasing discrepancy is a consequence of the use of separate models for what is in actuality a continuous and smooth variation. It is recommended that the larger of the two concentrations predicted around the matching distance be used for $t > t_e$.

III.3 Instantaneous Spills in Steady and Tidal Rivers

III.3.1 General Description of Model

The overall model is composed of very near-field, near-field, intermediate-field, and far-field sub-models. In the very near-field, the dilution of the spilled chemical is caused primarily by buoyancy-induced mixing. (The initial momentum included in the corresponding sub-model for a continuous spill is considered negligible here.) The near-field sub-model treats the dilution due primarily to turbulent diffusion after the initial buoyancy has been dissipated. Once the concentration becomes nearly uniform over the channel depth, the intermediate-field sub-model is used to include longitudinal dispersion as well as lateral diffusion. Finally, the far-field sub-model treats the longitudinal dispersion of the spill after it has been mixed uniformly over the depth and width.

When the chemical is neutrally buoyant or nearly so, gravity-induced mixing is small. The very near-field model is not needed then, although the spill is still assumed to rise to the surface or sink to the bottom whenever its density is not identically equal to water.

In all cases, the various sub-models are matched by a procedure that ensures that the peak concentration is continuous in time and distance and that conserves the spilled mass.

The models for a tidal river are the same in form as those for a steady river. There are differences, however, in the correlating equations used for the diffusion and dispersion coefficients.

III.3.2 Buoyancy-Induced Mixing Regime

Available models of the dilution of a heavy gas into the atmosphere [14,15] are adapted here to treat the initial mixing of a spill that has a density significantly different from water. A heavier-than-water chemical spilled into water should, in fact, respond like a heavy gas spilled along the ground. For a lighter-than-water chemical, the analogy

is not exact since turbulent friction at the free surface resembles only qualitatively that of a gas spreading along the ground; nonetheless, the dense cloud models represent the most realistic models available at this time.

In order to provide a starting condition, the initial shape of the cloud is assumed to be cylindrical, primarily because an axisymmetric flow is assumed in the dense cloud models. Any more exact description of the shape would depend upon the puncture geometry, the actual (short) time required for the spill, and other factors that may not always be available. The spreading would rapidly become axisymmetric, in any case. For definiteness, the initial height, h_o , is assumed to be equal to the initial diameter; thus:

$$h_o = d_o = (4 M_o / \pi \rho_c)^{1/3} \quad (\text{III.53a})$$

If h_o is greater than the channel depth, it is changed and made equal to the depth; d_o is then re-computed as:

$$d_o = (2 M_o / \pi \rho_c d)^{1/2}; \quad h_o = d \quad (\text{III.53b})$$

(If d_o is of the order of magnitude of half the channel width, the spill is probably too large to be considered instantaneous. The spill description should be changed to continuous with a short discharge time.)

In order to determine whether buoyancy-induced mixing is important relative to turbulent diffusion, the initial gravity-wave velocity of the spill is compared to the friction velocity:

$$1.3 (g h_o |1 - \rho/\rho_c|)^{1/2} \geq 3.7 u_* \quad (\text{III.54})$$

The factor of 3.7 multiplying u_* has been derived from the test program described in Section V of this report. If Equation (III.54) is not satisfied, buoyancy-induced mixing will be small, and the very near-field sub-model is not needed. (The gravity-wave velocity is based on the absolute value of the density difference so that both positive and negative buoyancy can be treated.)

The chemical is assumed to fall to the channel bottom or rise to the top without dilution, and moves downstream at the river velocity during the rise or fall. Since the distance and time involved in this initial motion is small compared to the subsequent dilution time and the total distance the cloud moves, the error in this approximation is small.

The mixing analysis assumes a "top hat" concentration profile, in which the concentration is the same throughout the cloud and falls discontinuously to zero at the boundaries [14,15]. The basic computing equations are discussed below with the aid of Figure III.4a

Cloud Thickness

$$h_c = (M + M_w) / \pi \rho_{mix} r_c^2 \quad (\text{III.55})$$

Here, M is the mass of chemical remaining in the water at any time, and M_w is the mass of entrained water. When the cloud radius r_c exceeds the distance to either channel wall, the part predicted to be outside the channel is reflected back on the cloud, and the average thickness is increased accordingly.

Cloud Radius

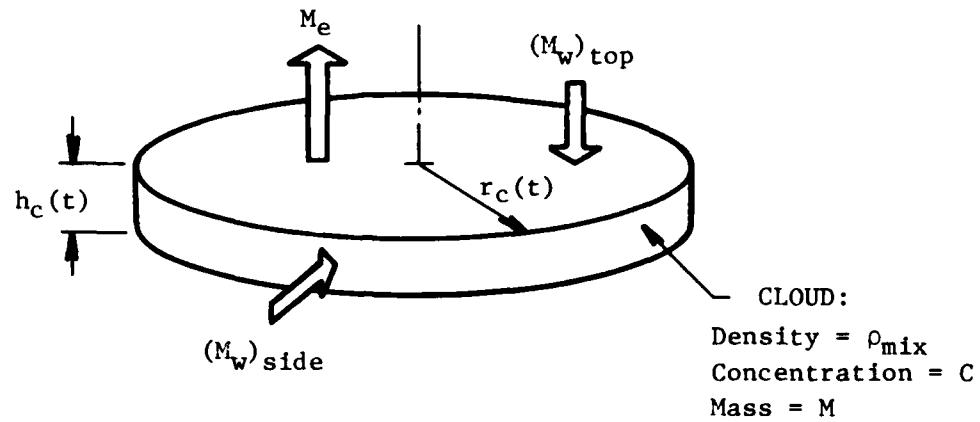
The radius of the cloud increases because of buoyancy-induced spreading:

$$\frac{dr_c}{dt} = 1.3 (gh_c | 1 - \rho/\rho_{mix} |)^{1/2} \quad (\text{III.56})$$

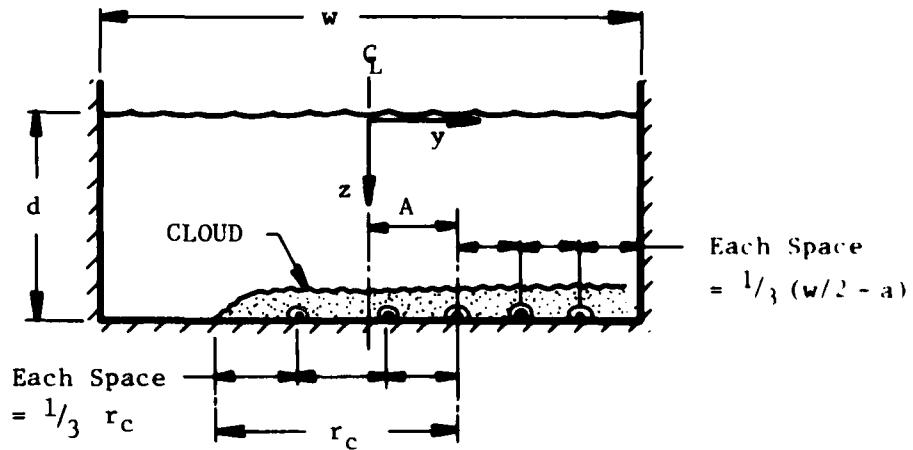
where $r_c = d_o/2$ at time $t = t_o$ = the time duration required for the cloud to sink to the bottom or rise to the surface after the spill occurs.

Water Entrainment Velocity

Water is entrained around the sides of the cloud and across the flat surface exposed to the water, which for convenience will be called



a. Schematic of Buoyant Cloud



b. Location of Point Sources

FIGURE III.4 DETAILS OF INSTANTANEOUS SPILL MODEL.

the top. The entrainment around the sides is referenced to the area of the top; thus, the entrainment is:

$$\frac{dM_w}{dt} = \pi \rho r_c^2 [u_{top} + 2 (h_c/r_c) u_{side}] \quad (\text{III.57})$$

where $M_w = 0$ at time $t = t_0$. When r_c exceeds the distance to either wall, only the part of the cloud area within the channel is used to compute dM_w/dt .

The entrainment velocity around the sides is proportional to the gravity-wave velocity:

$$u_{side} = 2 [c_f (dr_c/dt)]^2 / (dr_c/dt)_{t=t_0} \quad (\text{III.58a})$$

The friction coefficient $c_f = 3.807 n/R_h^{1/6}$ is computed in accordance with the definition of friction velocity u_* for a channel flow, Equation (III.30), rather than for a gas flow over the ground; this change of definition is one of the main differences between the available dense gas cloud models and the instantaneous chemical spill model. The entrainment velocity over the top surface is

$$u_{top} = 1.3 u_* / (6.0 + 0.25 N_{Ri}) \quad (\text{III.58b})$$

Ordinarily, the entrainment is dominated by u_{top} .

The Richardson number appearing in Equation (III.58b) is defined in accordance with [15]:

$$N_{Ri} = 0.59 (dr_c/dt)^2 / (1.3 u_*)^2 \quad (\text{III.59})$$

The numerical value of the denominator of the u_{top} prediction recommended in [15] is $3.33 + 0.29 N_{Ri}$. But when the model predictions were compared to the test results described in Section V of this report, it was found that the recommended form overpredicted the entrainment rate, and the magnitude of the denominator had to be increased. It also appeared that the stabilizing influence of stratification (i.e., Richardson number) was over-emphasized by

the recommended form, and its relative influence was therefore diminished in the form used here; the evidence for this effect, however, is not as strong as that for the overall magnitude of the denominator.

In all these equations, u_* is based on the velocity of a steady river or on the square root of the sum of the squares of the steady and oscillating components of a tidal river. There is some theoretical justification [5] for the choice used here for a tidal river.

Chemical Evaporation Rate

When the spilled chemical is lighter than water, the cloud, which is at the free surface, may evaporate at a rate

$$\frac{dM_e}{dt} = \pi \rho_c^2 H C \quad (\text{III.60})$$

where $M_e = 0$ at $t = t_0$. H is the mass transfer coefficient (see Appendix B). The mass of chemical remaining in the water is then

$$M = M_0 - M_e \quad (\text{III.61})$$

For heavier-than-water chemicals, there is no evaporation.

Mixture Density

The volume of the cloud is assumed to be equal to the individual volumes of unmixed chemical and water; that is, the chemical is passive and the total volume is unchanged by mixing. Thus:

$$\rho_{\text{mix}} = (M + M_w) / (M/\rho_c + M_w/\rho) \quad (\text{III.62})$$

Cloud Concentration

The same assumption used for Equation (III.62) gives the concentration as:

$$C = M / (M/\rho_c + M_w/\rho) \quad (III.63)$$

Cloud Location

The center of the cloud lies at the surface or channel bottom (depending on whether ρ_c is less than or greater than ρ) and at a downstream location equal to:

$$x = \int_0^t (u) dt \quad (III.64)$$

Termination of Buoyancy-Induced Mixing

At some point the mixture density approaches the water density so closely that buoyancy-induced mixing becomes negligible. (Note from Equations (III.62) and (III.63) that the concentration can still be large even when $\rho_{mix} \approx \rho$.) By comparing model predictions to test data, it was found that a reasonable cut-off criterion was the time when

$$\frac{dr_c}{dt} = 3.7 u_* \quad (III.65)$$

was first satisfied. (Equation (III.54) follows from this correlation.)

Equations (III.53) ~ (III.65) completely describe the dilution caused by buoyancy-induced mixing. In practice, the set of coupled differential and algebraic equations must be solved numerically. Some further details are given in Appendix B.

III.3.3 Diffusion-Dispersion Mixing Regimes

Downstream of the buoyancy-induced mixing regime, the spill is diluted by turbulent mixing (the near-field sub-model), then by a combination of turbulent mixing laterally and dispersion longitudinally (the intermediate-field model), and finally by turbulent dispersion (the far-field model).

Near-Field Model

If the spill is predicted to have a buoyancy-induced mixing phase, the cloud will usually be thin and wide by the time Equation (III.65) is satisfied (see Figure III.4b). A single point source is not a valid representation of the subsequent mixing by turbulent diffusion. Perhaps the most logical form of near-field sub-model would be a horizontal line source with a length equal to the cloud width. Such a representation has the disadvantages, however, that (1) it would not reproduce the mixing of a neutrally-buoyant spill, for which a point source is the best near-field representation, (2) it would be a clumsy representation if the cloud width was small relative to the channel width, and (3) separate computational forms would be needed for buoyant and non-buoyant spills. A good compromise choice is thus to represent the near-field as a set of point sources spread out horizontally along the spill width; then, if the spill is neutrally-buoyant, the number of point sources can easily be reduced to one. In the computerized model, five point sources are used, two on each side of the spill location spaced out at distances one-third of the way to the spill boundary (either r_c or the channel wall) and one at the spill location; four first-order images for each point source are also included.

The computing equation for the near-field sub-model [5] is thus:

$$C(x, y, z, t) = \sum_{n=1}^N \frac{(M/N) \exp [-(x - \bar{u}t)^2 / 4 \epsilon_x t]}{(4\pi t)^{3/2} (\epsilon_x \epsilon_y \epsilon_z)^{1/2}} \times$$
$$\sum_{n=1}^5 \exp [-(y - y_n)^2 / 4 \epsilon_y t - (z - z_n)^2 / 4 \epsilon_z t] \quad (\text{III.66})$$

with $N = 5$ for a buoyant spill and $N = 1$ for a non-buoyant one. The outer summation is meant to indicate that there are N sets of point sources and images. The symbol $\bar{u}t$ is shorthand for the integral

$$\int_0^t u \times dt$$

Intermediate-Field Model

For a buoyant spill, five line sources are used to represent the intermediate-field, each at a position corresponding to one of the five point sources; for a non-buoyant spill, one line source is used at $y = a$. The computing equation is:

$$C(x, y, t) = \sum_{n=1}^N \frac{(M/N) \exp [-(x - \bar{u}t)^2/4 e_x t]}{(4\pi e_x t)^{1/2} w d} \left\{ 1 + \frac{(x - \bar{u}t)^2}{4 e_x t} \left(\frac{e_t}{e_x} \right) \right\} \times \\ \left\{ 1 + 2 \sum_{n=1}^{\infty} \cos \left(\frac{m\pi w_s}{w} \right) \cos \left[\frac{m\pi(y + w/2)}{w} \right] \exp \left[-\frac{m^2 \pi^2 e_y x}{w^2} \right] \right\} \quad (\text{III.67})$$

where w_s is the sum of $w/2$ and the y -coordinate distance to the line source in question; again $N=1$ for a non-buoyant spill and $N=5$ for a buoyant one. The first set of curly brackets accounts for the tidal flow, in which e_t is the time-varying part of the dispersion coefficient. (If there is no tidal flow, $e_t = 0$ and the equation reduces to the steady flow form [12].) As shown in Appendix B, the time-averaged dispersion coefficient is:

$$e_x = (5.93 du_*) \left\{ 1 + \frac{1}{2} (\epsilon_z T/d^2) / [\pi^2/4 + (\epsilon_z T/d^2)^2]^{1/2} \right\} \quad (\text{III.68})$$

which reduces to the standard form for a steady river when the tidal period $T = 0$. The time-varying dispersion coefficient is

$$e_t = \frac{1}{4} (5.93 du_*) \left(\frac{(\epsilon_z T/d^2)}{[\pi^2/4 + (\epsilon_z T/d^2)^2]^{1/2}} \times \right. \\ \left. \left\{ \sin \left[\frac{2\pi}{T} (t + \alpha) + \theta \right] - \cos \left[\frac{4\pi}{T} (t + \alpha) + \theta \right] \right\} \right. \\ \left. + 4 \sin \left[\frac{2\pi}{T} (t + \alpha) \right] \right) \quad (\text{III.69})$$

where

$$\theta = -\arcsin [(\pi^2/4)(\epsilon_z T/d^2)^2 + 1]^{-1} \quad (\text{III.70})$$

These relations are based on a tidal velocity of the form

$$u = u_0 + u_1 \sin \frac{2\pi}{T} (t + \alpha) \quad (\text{III.71})$$

where α is a phase shift that is selected to allow the spill to occur at $t = 0$.

Far-Field Model

In the far-field, longitudinal dispersion acts to dilute the spill, which is now mixed uniformly over the cross-section. The computing equation [5] is:

$$C(x, t) = M \exp [-(x - \bar{u}t)^2 / 4 E_x t] \times \left\{ 1 + \frac{(x - \bar{u}t)^2}{4 E_x t} \left(\frac{E_t}{E_x} \right) \right\} / \text{wd} (4\pi E_x t)^{1/2} \quad (\text{III.72})$$

E_x and E_t are of the same form as e_x and e_t , Equations (III.68) and (III.69), except that the factor $5.93 du_*$ is replaced by $0.18 (u_* u)^{1/2} w^2 / R_h$, where $u = (u_0^2 + u_1^2)^{1/2}$.

III.3.4 Matching of Models

It was indicated in Section III.3.2 that the very near-field model is used to compute the spill concentration up to the time that dr_c/dt first equals $3.7 u_*$. Afterwards, the concentration is computed by the near-field model. In order to insure that the peak concentration is a continuous function of time and distance, a fictitious virtual origin must be selected for the near-field model. This matching procedure is accomplished iteratively in the computerized model by determining a total time duration t_{ONF} that, when used in Equation (III.66), gives a peak concentration equal to that of the very near field. (Note that $x - \bar{u}t = 0$ at the location of the peak concentration.) Letting t_{VNF} be the time required for $dr_c/dt = 3.7 u_*$, the virtual origin of the near-field model is shifted forward in time by an amount

$$\Delta t_{NF} = t_{VNF} - t_{ONF} \quad (III.73)$$

There is a corresponding downstream shift Δx_{NF} of the x-coordinate origin by the amount

$$\Delta x_{NF} = \int_0^{\Delta t_{NF}} (u) * dt. \quad (III.74)$$

At a given observation point, the values of x and t used in the near-field model are taken as $x - \Delta x_{NF}$ and $t - \Delta t_{NF}$.

If the spill is neutrally buoyant, so that a very near-field model is not needed, t_{ONF} is determined to match a concentration equal to ρ_c . The virtual origin is then shifted backward in time by the same amount t_{ONF} .

Using a similar procedure, a virtual origin is found for the intermediate-field model by matching its concentration to the depth-averaged near-field concentration computed at the time when the predicted near-field concentration is nearly uniform over the depth; that is, at the time when $t = 0.3 d^2/\epsilon_z$. Likewise, a virtual origin for the far-field model is found by matching its concentration to the width-averaged intermediate-field concentration computed at $t = 0.3 w^2/\epsilon_y$.

III.4 Continuous Spills in Tidal Rivers

III.4.1 General Description of Model

This model is based on sub-models and matching procedures similar to those described in Section III.2 for a continuous spill in a steady river. There are, however, three major differences: (1) the dispersion coefficients are allowed to vary with the tidal flow; (2) for large tides, the river is allowed to flow back-and-forth under the spill site, accumulating more chemical with each pass; and (3) most importantly, buoyancy-induced spreading and mixing are not included. The implication of the last difference is that mixing is not accurately predicted in the very near-field for chemicals substantially heavier or lighter than water. Although the model therefore is

more limited in scope than the others, the time-dependent variation of source size and strength that would be needed in a Colenbrander type of model makes it unfeasible to treat buoyancy-induced mixing analytically. The very near-field model thus includes only the buoyancy and momentum effects of the initial plume (i.e., Ooms' model).

In the discussion below, the near-, intermediate-, and far-field models are given in complete time-dependent form, as summarized from the original analysis detailed in Appendix C.* The computerized form of the model follows from the time-dependent equations; but, in order to facilitate the matching of the various sub-models, the tidal period is broken up into six segments, in each of which the current is assumed constant and equal to its time-average value, and the computerized sub-models actually are based on these time-average currents. Concentration distributions for any specified duration are then built-up by combining the appropriate numbers of each of the sub-models.

III.4.2 Jet Buoyancy-Momentum Regime

The very near-field model treats the initial dilution of the jet of chemical exiting the puncture caused by its buoyancy and momentum. The time required by a fluid particle in this plume to travel from the puncture to the location where the initial buoyancy and momentum have been dissipated or to where the plume intersects a channel boundary is short compared to a tidal period. Thus, the effect of a time-varying current on the plume dynamics is negligible, and Ooms' formulation [3] can be used as though the current was steady. In theory, an infinite number of such steady models would be needed to predict the dilution at every instant of a tidal cycle. To keep the amount of computations to a manageable level, the tidal cycle is broken up into a small number of segments (six, in the computerized model) in each of which the current is taken as steady at its average value. The model of

* Near the end of the present work, it was discovered that a somewhat similar analysis of the far-field had been published in 1982 [16].

buoyancy-momentum mixing in the very near-field for any of these periods is, consequently, the same as that described in Section III.2.2. Details of the analytical development will not be repeated here.

III.4.3 Diffusion-Dispersion Regimes

In the near-field, the spill is diluted primarily by turbulent diffusion, and the concentration varies considerably over both the depth and width of the channel. The appropriate model for this kind of mixing is a point source, with images to account for the channel boundaries. A point source model of a continuous spill can be developed readily by integrating over time the concentration due to a stream of infinitesimal instantaneous point-source spills [5]. As shown in Appendix C, the result is:

$$C(x, y, z, t) = \sum_{j=1}^P \left[\frac{\dot{M} \bar{u}_j}{4\pi x (\varepsilon_y \varepsilon_z)^{1/2} |u_j|} \right] \times \left\{ \sum_{n=1}^5 \exp \left[- (y - y_n)^2 \bar{u}_j / 4x \varepsilon_y - (z - z_n)^2 \bar{u}_j / 4x \varepsilon_z \right] \right\} \quad (\text{III.75})$$

Here, \bar{u}_j is the time-average current over the period $(t - t_j)$ required for the water that was at the spill site ($x = 0$) at time t_j to reach the observation point x at the time t , and $|u_j|$ is the magnitude of the current at time t_j . For large tides, the current may reverse direction, so the water at the observation point at the time t may have passed under the spill site more than once; the number of such reversals up to the observation time is denoted by P in Equation (III.75).

The current, as explained in Section III.3, is of the form $u = u_0 + u_1 \sin [2\pi (t + \alpha)/T]$. Thus, the times t_j are the roots of the equation $x - \int u \cdot dt = 0$, where the limits on the integral are t and t_j ; thus,

$$x - u_0(t - t_j) + \frac{u_1 T}{2\pi} \left[\cos \frac{2\pi}{T} (t + \alpha) - \cos \frac{2\pi}{T} (t_j + \alpha) \right] = 0 \quad (\text{III.76})$$

which must be solved numerically for the P roots. The time-average current is

$$\bar{u}_j = u_0 - \frac{u_1 T}{2\pi(t-t_j)} \left[\cos \frac{2\pi}{T} (t+\alpha) - \cos \frac{2\pi}{T} (t_j + \alpha) \right] \quad (\text{III.77})$$

and $|u_j|$ can be computed by taking the absolute value of u evaluated at $t = t_j$.

In order to examine the implications of Equation (III.75) it is convenient to assume that $P = 1$ so that current reversals need not be considered. By comparing Equation (III.75) to Equation (III.27) of Section III.2.4, it can be seen that the concentration of chemical in a tidal river differs from that in a steady river having the same average current by the factor $\bar{u}_j / |u_j|$. For a steady river with a relatively slow current, the amount of chemical injected into the water (per unit volume of water) is relatively large; but the time required for the chemical to be transported to the observation point is long, thus allowing a relatively long time for dilution. The opposite occurs when the current is relatively fast. Therefore, the total dilution along the centerline of the spill is the same in all cases (except for the effect of images) and the distribution depends only on the distance to the observation point. For a tidal river, the current can be slow as the water passes by the spill site but can have a higher average value as it transports the chemical to the observation point; less dilution would therefore occur than for a steady river. Likewise, the dilution will be greater when \bar{u}_j is smaller than $|u_j|$. Equation (III.75) shows, in fact, that the ratio of the centerline dilution of a tidal river and a steady river is just $\bar{u}_j / |u_j|$.

When $|u_j|$ is very small compared to \bar{u}_j , the analysis leading to Equation (III.75) is not valid. Longitudinal diffusion, which was neglected in the analysis, is an important dilution mechanism for the highly non-uniform longitudinal distributions of chemical that occur for such a condition. The concentration does not, therefore, become large in proportion to $\bar{u}_j / |u_j| \gg 1$, as Equation (III.75) implies. By taking longitudinal diffusion into account whenever $u_j \approx 0$, it is found that the expression

within square brackets in Equation (III.75) should be selected as the minimum of the following three possibilities:

$$\dot{M} \bar{u}_j / \{4\pi x (\epsilon_y \epsilon_z)^{1/2} |u_j| \}$$

or

$$2.6 \dot{M}^{1/2} \bar{u}_j^{5/4} / \{4\pi (4\pi \epsilon_y \epsilon_z)^{1/2} x^{5/4} \epsilon_x^{1/4} u_1^{1/2} [\cos \frac{2\pi}{T} (t_j + \alpha)]^{1/2} \}$$

or

$$1.86 \dot{M}^{2/3} \bar{u}_j^{4/3} / \{4\pi (4\pi \epsilon_y \epsilon_z)^{1/2} x^{4/3} \epsilon_x^{1/6} u_1^{1/3} [\sin \frac{2\pi}{T} (t_j + \alpha)]^{1/3} \}$$

(The last form is necessary to treat cases when not only $u_j \approx 0$, but also $\cos [2\pi (t_j + \alpha)/T] \approx 0$.) The first, original, expression applies to the majority of cases.

In the intermediate field, a similar integration of infinitesimal line sources gives:

$$C(x, y, t) = \sum_{j=1}^p C_j \left\{ 1 + 2 \sum_{m=1}^{\infty} \cos \left(\frac{m\pi w_s}{w} \right) \cos \left[\frac{m\pi (y + w/2)}{w} \right] \times \exp \left(-m^2 \pi^2 e_y x / w^2 \bar{u}_j \right) \right\} \quad (III.78a)$$

where C_j is the minimum of the following three possibilities:

$$\dot{M} / wd |u_j| \quad (III.78b)$$

or

$$5.2 \dot{M}^{1/2} / wd (x \bar{u}_j)^{1/4} e_x^{1/4} [4\pi \cos \frac{2\pi}{T} (t_j + \alpha)]^{1/2} \quad (III.78c)$$

or

$$3.72 \dot{M}^{2/3} / wd x^{1/3} e_x^{1/3} [4\pi \sin \frac{2\pi}{T} (t_j + \alpha)]^{1/3} \quad (III.78d)$$

Here, e_x is the time-average dispersion coefficient given previously in Equation (III.68). The first expression applies to the majority of cases.

In the far-field, the concentration is

$$C_3(x,t) = \sum_{j=1}^M \bar{C}_j \quad (\text{III.79})$$

Here, \bar{C}_j is the same in form as C_j but with e_x replaced by E_x (see Equation (III.72)).

III.4.4 Matching of Models

Exactly as for the models of a continuous spill in a steady river, the various models are matched at the limits of their range of validity to insure that the peak concentration is a continuous function of time and downstream distance. In theory, the matching times and distances (i.e., virtual origins) are themselves functions of time and distance. In practice, for the computerized model, the tidal cycle is broken up into six segments, models are developed for each segment using the time-average currents, and the six sets of models are then matched as for a steady river. Since the tide is periodic, spills of any specified duration can then be treated by using the six sets of models repetitively.

III.4.5 Concentration Models After Discharge Ceases

After the chemical discharge ceases at time t_e , the spill translates downstream and is gradually diluted further by longitudinal dispersion (which accomplishes this by increasing the total river length affected by the spill). Because of the time-varying current, analytical methods of predicting the concentration after the spill ceases, such as were described for a steady river, are not tractable. Instead, it is argued that at any given observation point in the spill, diffusion and dispersion of the chemical will proceed at almost the same rate as when the spill was continuing. The result is that the observer will continue to experience the same concentration

that was present at the observation point during the spill, until the entire affected region has passed by. After that, the concentration will be zero. This procedure will slightly overestimate the concentration and slightly underestimate the total length of the spill in the river.

For an observation point downstream of the spill at the time the discharge stops, the concentration is assumed to be zero until the leading edge of the affected region reaches that location. Depending upon this downstream distance, the leading edge might represent an intermediate-field or a far-field concentration. If the discharge time is sufficiently long, the leading edge will represent a far-field, and by the same logic outlined above, all the downstream observation points will continue to be in the far-field until the entire spill passes. Otherwise, some downstream points will lie in the intermediate-field and some, even further downstream, will lie in the far-field. This kind of possibility is treated by switching to the far-field model for any observation time t greater than $0.3 w^2/e_x$, which is approximately the length of time required for lateral diffusion to mix the spilled chemical uniformly across the channel width.

III.5 Spills in Estuaries and Bays

The models presented in Sections III.2, III.3, and III.4 are all based upon the idealization of a constant width, constant depth channel having a well defined flow direction. For estuaries and bays, that idealization is untenable. Each case must be treated individually, with the boundaries explicitly included in the description and the various flows computed as part of the model. A generalized model that can perform such calculations, the Dynamic Estuary Model [17], is already available and is recommended for use in such cases.

The Dynamic Estuary Model (DEM) is structured conceptually for a specific system as a single-dimensioned network approximation of a vertically mixed system of interconnected channels and embayments. It is composed of two modules: a hydrodynamic module and a transport module. The hydrodynamic module solves a set of motion equations written for the channels of the network system and a set of continuity equations for the embayments. The

solution yields a temporal description of the flow and velocity in each channel and the water surface elevation at the center of each embayment. Using the hydrodynamic output as the driver, the transport module computes the mass transport of specified constituents into and out of each embayment due to convection and diffusion and/or dispersion with first order reaction kinetics accounted for within each embayment. Solutions within the transport module give the temporal or intratidal variations of concentration and the tidally averaged concentrations at the center of each embayment.

The basic approach for application of the DEM to a specific estuary involves the discretization of the system into a series of volumetric units or embayments called "nodes" connected by a system of flow elements or channels called "links". Figure III.5a is a conceptual layout of links for a generalized estuary, and Figure III.5b illustrates the nodes whose volumes for the most part are made up of the half volumes of the connecting links. Typically, nodes can be of any polygonal shape with the node spacing set by the scale of the problem and the geometry of the problem. Nodes are characterized by their volumes (usually equal to half volumes of the connecting links), surface areas, depths, and water surface elevations. In addition, for the transport module, first order reaction coefficients as required are associated with nodes. Constituent mass and concentration are identified with the system nodes.

Flows in the DEM are allowed to occur between nodes along the connecting links. Each link is described by its length, depth or hydraulic radius, surface width, cross-section or flow area, and roughness. For computation of the transport mechanisms, either diffusion or dispersion coefficients are assigned or computed for each link in the system.

Time and space scales are both important in the DEM. Not only must they be selected to represent adequately the system geometry, tidal action, and hydrologic characteristics of the estuary, but they must be such to characterize properly the spill and its movement in a two-dimensional sense. The DEM has the option to include more detail in specific areas of interest by the addition of more, but shorter, channels at any location. The finer detail, however, will only come at the expense of added computational effort.

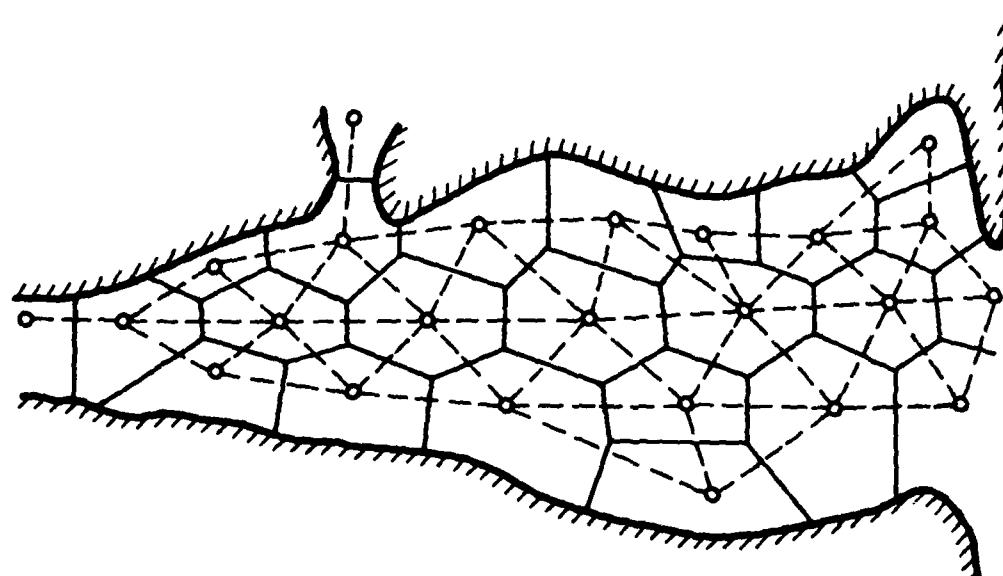
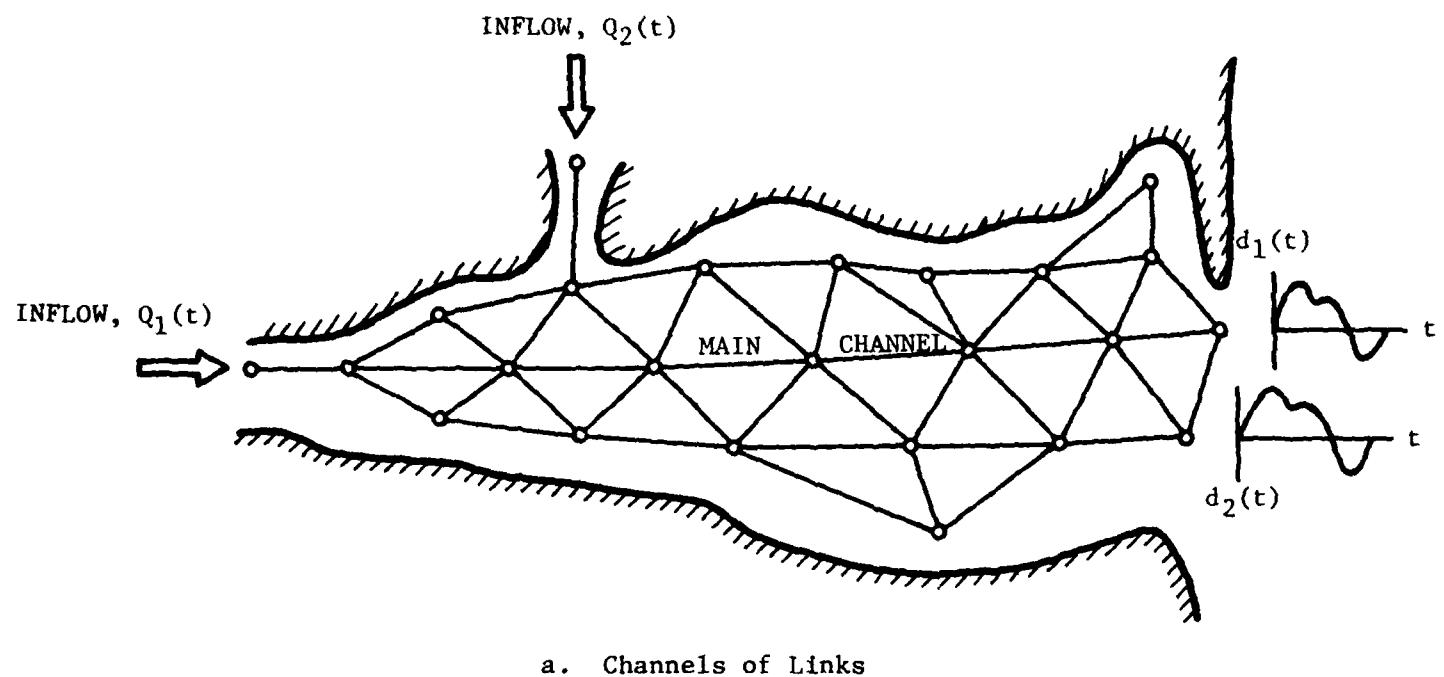


FIGURE III.5 DEM SYSTEM CONCEPTUALIZATION

The selection of scales may also be directly relevant to the time over which the transport phenomenon is observed.

The hydrodynamic module of the DEM provides for the computation of tidal flows and water surface elevation in what is effectively a one-dimensional representation of a two-dimensional system. The main limitation of the DEM is that it is limited to estuaries wherein vertical stratification is virtually absent and tidal velocities can be handled in a depth-integrated manner. While this is a major constraint in some systems, the dominant motions in most estuaries are in the horizontal plane; and in many shallow estuaries, wind, waves, and other mixing effects preclude the formation of strong stratification. Even in many deep channels with heavy ship traffic, displacement effects of loaded vessels and wheel water provide a "stirring" such that stratification occurs only when accidents shut down shipping or floods occur from upland sources.

A significant amount of effort is needed for each use of the estuary model. It is probably not suitable, then, for the evaluation of rapid responses unless a library of models has already been assembled for all the estuaries and bays of potential interest to the Coast Guard. The DEM should also be modified to allow instantaneous spills; the efforts needed to make such a modification are anticipated to be relatively small. It is unlikely, however, that the DEM can be modified to predict buoyancy- or momentum-induced mixing and other very near-field effects.

IV. EXPERIMENTAL DESIGN AND DATA COLLECTION

IV.1 Experimental Design

The purpose of the experimental design was to develop a test plan for a series of experiments that would provide the data necessary for validating the revised models for both continuous and instantaneous spills. The design process involved several independent steps that had to be performed before the final test plan could be executed. These were:

- o Definition of test program objectives
- o Performing a model sensitivity analysis
- o Selection of modeling criteria for scale model tests
- o Definition of the test plan.

The work carried out in each of these elements is described in the following sections.

IV.1.1 Test Program Objectives

The main objective of the test program was to perform a set of experiments to quantify the effects of discharge momentum and buoyancy on the behavior of chemical plumes that result from instantaneous and continuous discharges of water soluble chemicals into a turbulent channel flow. The tests should be designed to include the influences of

- o specific gravity of the chemical (<1, ~1, and >1)
- o discharge flowrate (continuous spill)
- o discharge volume (instantaneous spill)
- o channel flow velocity
- o channel turbulence level.

The behavior of the chemical plume during the test program was to be determined through the use of

- o flow visualization (by adding soluble dyes to the chemical before discharge), and

- o measurement of the chemical concentration distribution in both the vertical and cross-stream directions at selected downstream stations.

The concentration profile data acquired during the test program were compared with predictions of concentration distribution from the revised computer models. The comparison of model predictions and experimental data were then used to re-evaluate best values for the empirical entrainment and dispersion coefficients that appear in the mixing and dilution models.

IV.1.2 Sensitivity Analysis

A sensitivity analysis was performed for the revised mixing and dilution models to determine the sensitivity of the predicted concentration distribution at downstream locations to changes in the values of the model variables. This technique is useful in determining which variables have the greatest influence on the concentration distribution, and need to be measured and controlled precisely during experiments. It will also indicate which variables (if any) have little influence on model predictions and can safely be omitted from the test program.

The sensitivity analyses were performed before the start of the laboratory test program. At that time, the need for Colenbrander's model to simulate the buoyant, gravity spreading of chemical plumes along the upper or lower river surface in the very near-field region was not recognized. Likewise, the model for mixing and dilution of instantaneous spills of buoyant chemicals did not include Eidsvik's model for gravity spreading and entrainment when the model sensitivity analysis was performed. Therefore, the results discussed in this section do not pertain entirely to the complete revised models described in Section III. Sensitivity analyses were performed for both continuous and instantaneous spills in steady and tidal rivers, but only the results for the continuous spill in a steady river are presented here, since the results of the instantaneous spill are very similar.

For each model, the change in maximum downstream concentration was computed for a $\pm 5\%$ change in value of each model variable

about a selected baseline condition. The sensitivity coefficient for each variable was determined as:

$$\Delta SC_x = (\Delta C/C_0) / (\Delta X/X_0) \quad (IV.1)$$

Here ΔC is the concentration change from C_0 for a ΔX change in the variable X_0 . When SC_x is positive, C increases as X increases and decreases when X decreases; the opposite holds when SC_x is negative. The magnitudes of SC_x indicates the sensitivity of the computed concentration to the selected value of X ; if $SC_x = 1.0$, for example, the percentage change in C is the same as the percentage change in X ; values of SC_x greater or less than one indicate greater or less sensitivity to changes in X .

Table IV.1 gives the results of the sensitivity analysis for the case of a chemical with a specific gravity of 1.2 spilled at a rate of $0.14 \text{ m}^3/\text{sec}$ into a river flowing steadily at a velocity of 1 m/s . The spill rate corresponds roughly to the emptying of a $10\text{m} \times 10\text{m} \times 20\text{m}$ tank in four hours. The peak concentrations at three downstream locations are given in the table; the 5m location is well within the "very near field" where both the buoyancy and the momentum of spilled material are important, the 500m location is in the "near field" region where buoyancy and momentum are no longer important but where the concentration still varies considerably over the depth and width of the river cross-section, and the 5000m location is in the region where the concentration over the depth, but not the width, is uniform. Note that physical parameters, such as spill rate, chemical density, river dimensions, etc., have been varied as well as numerical parameters, such as entrainment and dispersion/diffusion coefficients. The sensitivity coefficients given in the table are averages of the \pm calculations.

It can be seen that changes of the order of $\pm 5\%$ in the values of the model variable do not greatly affect the computed concentrations. This is a desirable result in the sense that obtaining exact values of the variables may be difficult in actual full-scale cases. (Some of the variables have an effect on the trajectory of the buoyancy/momentum jet, but the table only examines the peak concentrations, independently of where in the river cross-section they occur.) The very near-field concentration is fairly sensitive

TABLE IV.1 SENSITIVITY COEFFICIENTS FOR CONTINUOUS DISCHARGE
OF HEAVIER-THAN-WATER CHEMICAL IN A STEADY RIVER

- o Physical Parameters: Chemical density = 1200 kg/m³; Chemical flowrate = 0.14 m³/sec; Tank puncture diameter = 1.0 m; River dimensions = 200 m x 25 m; River current = 1.0 m/sec.
- o Spill Location: 70 m from bank/ 10 m below surface; jetting downward
- o Numerical Coefficients: River turbulence level = 15%; Plume cross-stream decay constant, λ = 1.690; Velocity entrainment coefficients, α_1 = 0.097, α_2 = 1.238; Turbulence entrainment coefficient, α_3 = 1.000; Plume drag coefficient, C_d = 0.3; Evaporation mass transfer coefficients = 0 Diffusion coefficients: for ϵ_y = 0.6, for ϵ_z = 0.067
- o Baseline Peak Concentrations
5m downstream: 36.39 kg/m³
500m downstream: 0.1278 kg/m³
5000m downstream: 0.04818 kg/m³

<u>Parameter Varied</u>	<u>Sensitivity Coefficients</u>		
	<u>5m</u>	<u>500m</u>	<u>5000m</u>
Chemical density \pm 5%	-1.65	1.04	1.00
Chemical flowrate \pm 5%	0.34	1.11	1.00
Puncture diameter \pm 5%	0.37	0.01	0.00
River width \pm 5%	0.00	-1.26	-0.56
River depth \pm 5%	0.00	-1.78	-1.46
River current \pm 5%	0.50	-1.34	-0.98
Spill lateral location \pm 5%	0.00	0.88	0.37
Spill vertical location \pm 5%	0.00	0.55	0.02
Spill jetting upward	$\Delta C/C_0 = 0.093$	$\Delta C/C_0 = -0.039$	$\Delta C/C_0 = 0.002$
Turbulence level \pm 5%	-0.037	-0.31	0.01
Entrainment coefficients:			
α_1 \pm 5%	-0.01	0.00	0.00
α_2 \pm 5%	-0.050	-0.11	0.01
α_3 \pm 5%	0.37	-0.17	0.01
Decay constant λ , \pm 5%	0.00	-0.20	0.00
Diffusion coefficients			
ϵ_y \pm 5%	0.00	-0.022	-0.39
ϵ_z \pm 5%	0.00	-0.17	0.13

to the chemical density, with the concentration increasing as the density approaches neutral buoyancy. Neutral buoyancy, for which buoyancy-induced mixing is absent, gives, incidentally, the maximum very-near-field concentrations, at least in comparison to densities which do not vary too much from neutral buoyancy. The concentrations at 500m and 5000m vary in the expected way. For example, the concentration far downstream approaches a value of \dot{M}/uwd , where \dot{M} is the mass release rate, w is the river width, d is the river depth, and u is the river current. Thus, changes in any of these parameters change the concentration accordingly. Likewise, changes in the location of the spill in the river affect the concentration by increasing or decreasing the influence of the boundaries. The jet was initially directed downward for the baseline case. The effects of an initial upward direction are given in the table in the form $\Delta C/C_0$, since a sensitivity coefficient can not be defined for this parameter.

Table IV.2 gives similar results for a lighter-than-water chemical. In general, the computed sensitivity coefficients are comparable to Table IV.1.

Figure IV.1 is a plot of the trajectory of the momentum/buoyancy plume for the baseline cases shown in Tables IV.1 and IV.2. The neutral stability case is also shown, although the trajectory for neutral stability is shown as a straight line for clarity.

IV.1.3 Scale Modeling Criteria for Laboratory Tests

It was desired to design a test plan that would assist in validating the mixing and dilution models for a set of laboratory conditions that simulate full-scale conditions as much as possible. The following set of full-scale conditions were defined to guide the experimental plan development.

River Conditions:

- o depth, about 12 meters (40 ft)
- o width, about 120 meters (400 ft)
- o fresh water, no salinity intrusion

TABLE IV.2 SENSITIVITY COEFFICIENTS FOR CONTINUOUS DISCHARGE
OF LIGHTER-THAN-WATER CHEMICAL IN A STEADY RIVER

- o All Parameters are the same as in Table IV.1, except the chemical density is 800 kg/m³

- o Baseline Peak Concentrations:

5m downstream = 27.11 kg/m³
500m downstream = 0.09621 kg/m³
5000m downstream = 0.03192 kg/m³

<u>Parameter Varied</u>	<u>Sensitivity Coefficients</u>		
	<u>5m</u>	<u>500m</u>	<u>5000m</u>
Chemical density \pm 5%	2.98	0.85	1.01
Chemical flowrate \pm 5%	0.36	-1.08	1.00
Puncture diameter \pm 5%	0.21	0.50	0.00
River width \pm 5%	0.00	-1.06	-0.56
River depth \pm 5%	0.00	-0.41	-1.54
River current \pm 5%	0.66	-1.33	-0.98
Spill lateral location \pm 5%	0.00	0.76	0.36
Spill vertical location \pm 5%	0.00	-0.74	0.04
Spill jetting upward	$\Delta C/C_0 = -0.072$	$\Delta C/C_0 = .096$	$\Delta C/C_0 = -0.006$
Turbulence level \pm 5%	-0.40	-0.30	-0.01
Entrainment coefficients:			
$\alpha_1 \pm 5\%$	-0.01	0.00	0.00
$\alpha_2 \pm 5\%$	-0.52	-0.21	0.02
$\alpha_3 \pm 5\%$	-0.36	-0.31	0.02
Decay constant λ , \pm 5%	0.00	-0.31	0.01
Dispersion coefficients:			
$\epsilon_y \pm 5\%$	0.00	-0.25	-0.39
$\epsilon_z \pm 5\%$	0.00	-0.18	0.13

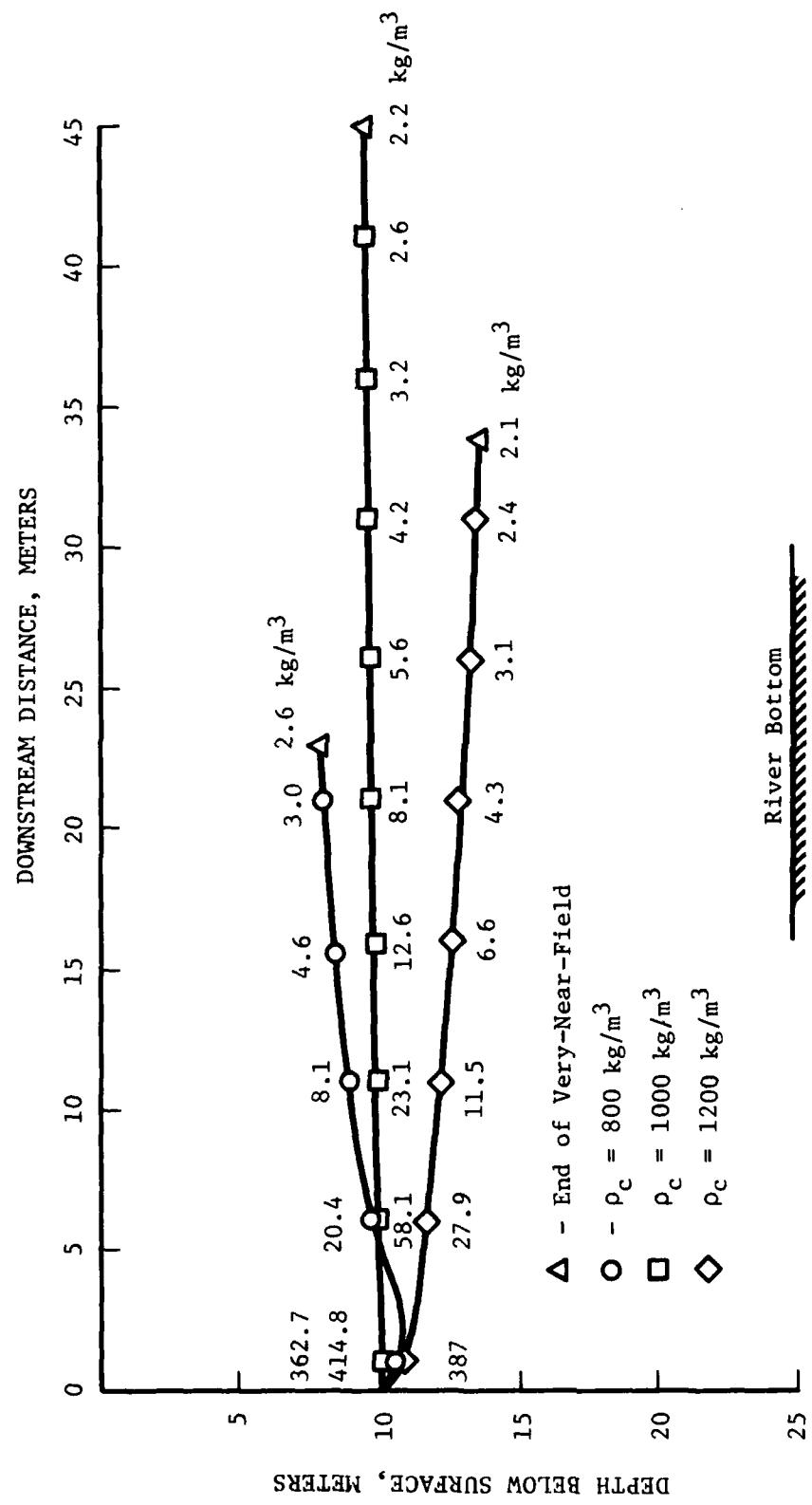


FIGURE IV.1 TRAJECTORY AND CONCENTRATION OF VARIOUS PLUMES

- o river velocity, 0.25 m/s to 1.0 m/s
- o shear velocity, nominally 5% to 10% of the river velocity.

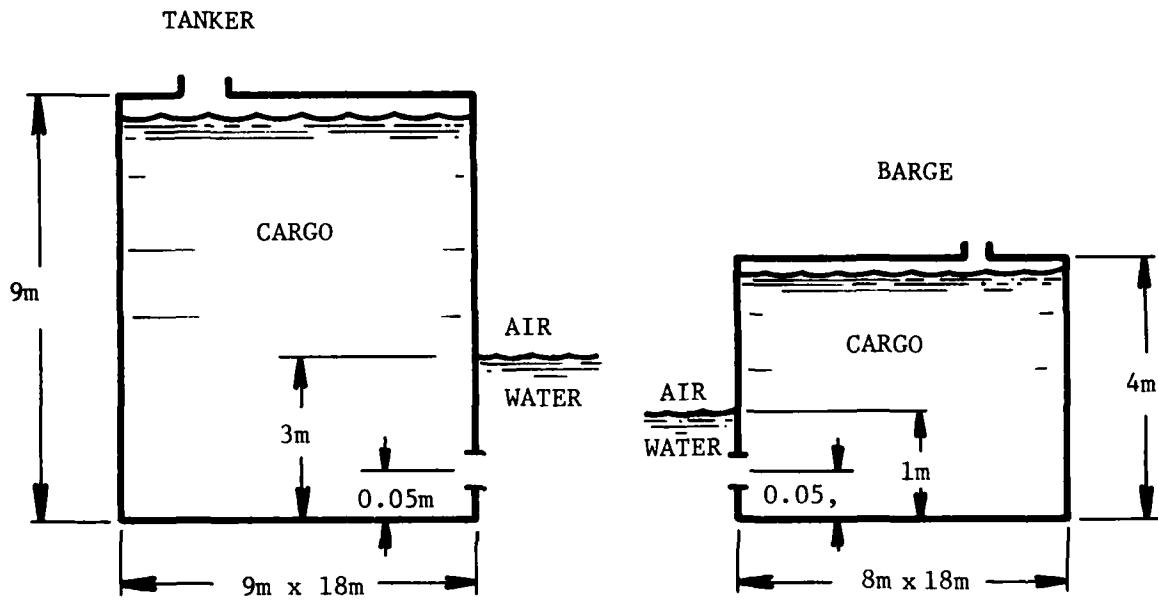
Spill Conditions:

- o chemical density gravity (relative to fresh water)
 - ~ 0.79 positive buoyancy
 - ~ 1.05 near neutral buoyancy
 - ~ 1.70 negative buoyancy
- o puncture diameter, nominally 0.5 meter
- o average spill velocity, 1 m/s to 4 m/s

To obtain the estimate of average spill velocity, the HACS venting rate model [6] was run to simulate both the discharge of cargo from a tanker and a barge, see Figure IV.2. The results showed that the discharge velocity and flow rate varied with time as the cargo level fell in the tank. It was particularly noted that the discharge velocity decreased considerably once water ingestion into the ruptured tank began. However, for the purposes of this project, an average discharge velocity was determined from the amount of cargo discharged and the elapsed time before water ingestion began. The values of discharge rate and discharge velocity are given in Table IV.3 for cargos with specific gravities of 1.7, 1.05, and 0.79. Note that the elapsed time before water ingestion begins is greater than 600 seconds (10 minutes) in every case. The values of discharge velocity ranged from 2 m/s to 4 m/s.

The mixing and dilution model for a continuous spill has three different flow regimes or development phases, the very near field (VNF), the near field (NF), and the far field (FF). In the VNF, momentum and buoyancy effects have a very strong influence on chemical plume trajectory and dilution. The list of important variables includes:

- o U velocity of spilled chemical
- o u local river velocity
- o ρ_c density of spilled chemical
- o ρ density of river water
- o D diameter of tank puncture
- o d local river depth
- o u_* shear velocity of river velocity profile



- Hole Size = 50 cm Diameter
- Discharge Coefficient, $C_D = 0.65$
- Tanks are 99% Full Initially

FIGURE IV.2 TANK AND CARGO GEOMETRY ASSUMED FOR DISCHARGE RATE CALCULATION USING HACS VENTING RATE MODEL

TABLE IV.3 RESULTS OF DISCHARGE RATE CALCULATION USING
HACS VENTING RATE MODEL [6]

Cargo Specific Gravity	AVERAGE VALUES OVER THE ENTIRE TANK DISCHARGE TIME				AVERAGE VALUES BEFORE WATER INGESTION BEGINS			
	Mass Discharged (kg)	Discharge Time (sec)	Discharge Rate (kg/sec)	Discharge Velocity (m/s)	Water Ingestion (sec)	Mass Discharged (kg)	Discharge Rate (kg/sec)	Discharge Velocity (m/s)
Tanker	1.70	2.440×10^6	137,520	17.74	0.053	1,502	1.945×10^6	1,295
	1.05	1.507×10^6	115,150	13.08	0.063	1,358	1.012×10^6	745
	0.79*	6.453×10^5	4,418	146.1	0.942	1,252	6.389×10^5	510
Barge	1.70	9.572×10^5	106,030	9.03	0.027	915.8	8.056×10^5	879
	1.05	5.911×10^5	61,967	9.54	0.046	848.0	4.394×10^5	518
	0.79*	2.989×10^5	5,186	57.64	0.372	802.6	2.932×10^5	365

* Cargo is left in the tank for these cases, because the ingested water fills up the tank from the bottom up and traps the remaining cargo.

- o θ_c orientation of chemical velocity vector, as it enters the river
- o ν viscosity of the water in the river.

Other factors of importance are:

- o Loaded depth of the tank
- o Location of the puncture on the hull
- o Height of the puncture above the water line, or
- o Depth of submergence of puncture below the water line.

These last four factors affect the venting rate of chemical from the tank puncture as a function of time.

Another factor of importance is the solubility of the chemical in water. When this project was begun, the lower limit of solubility was set at 1g/100cc of water. However, it was noted that several chemicals studied by Professor Thibodeaux at the University of Arkansas with solubilities in the range of 0.8 to 1.0 g/100 ml are very slow to mix with water and form spherical droplets when spilled into water [18]. The question of a proper lower solubility limit for use of the mixing and dilution model was discussed with the Coast Guard Technical Monitor and it was agreed that the lower limit of solubility should be increased to about 10g/100 ml based on the results of Thibodeaux's work.

The list of independent variables can be grouped into a set of dimensionless variables:

$$J = \frac{\rho_c U^2}{\rho u^2}$$

a ratio of the momentum of the spilled chemical to the local stream momentum.

$$Fr = \frac{\rho u^2}{(\rho_c - \rho)gd}$$

a densimetric Froude number which expresses the ratio of stream momentum to chemical buoyancy force

$$u_s/u$$

the ratio of shear velocity to stream velocity. This ratio affects the turbulent entrainment of the chemical plume by the river.

$$D/d$$

a length scale expressed as the ratio of puncture diameter to river depth.

ud/v

a Reynolds number based on river properties.

Of these five dimensionless variables, we expected that the first three would be of primary importance. The length scale factor D/d affects the size of the plume relative to the river. Larger values of D/d will require an earlier transition to the NF model when the plume diameter reaches a size approximately equal to the river depth. The Reynolds number is an important factor in determining whether a channel flow is laminar or turbulent. All dispersion experiments were conducted at a Reynolds number large enough to ensure turbulent entrainment.

For a proper simulation of full-scale conditions in laboratory scale experiments, the full-scale and model scale values of J , Fr , u_*/u , and D/d must be equal. For the laboratory simulation the following experimental chemicals were used:

- o ethanol (s.g. ~ 0.79)
- o sucrose (sugar water) (s.g. ~ 1.05)
- o sodium silicate (water glass, s.g. ~ 1.1 to 1.7)

which have specific gravities spanning the range of interest. Since the laboratory experiments were performed in reduced scale, Froude number equality required that velocity and time be scaled in the following way.

The ratio of river depth in full-scale (fs) to depth in model-scale (ms) is denoted by

$$\lambda = d_{fs}/d_{ms} \quad (IV.2)$$

Froude number equality requires

$$Fr = \left[\frac{\rho u^2}{(\rho_c - \rho)gd} \right]_{fs} = \left[\frac{\rho u^2}{(\rho_c - \rho)gd} \right]_{ms} \quad (IV.3)$$

since $[\rho_c/\rho]_{fs} = [\rho_c/\rho]_{ms}$, and g , the acceleration of gravity, is the same in model and full scales; thus,

$$\frac{[u^2]_{fs}}{[u^2]_{ms}} = \frac{[d_{fs}]}{[d_{ms}]} = \lambda \quad (VI.4)$$

This scale ratio holds true for all other velocities such as U and u_* as well.

Since velocity has the units of length divided by time, and the ratio of full scale length to model scale length is λ , we infer that the ratio of full scale time to model scale time is $\lambda^{0.5}$:

$$t_{fs} / t_{ms} = \lambda^{0.5}$$

This ratio was helpful in guiding the duration of averaging times for concentration samples and plume trajectory measurements.

A consideration of important variables for the instantaneous spill simulations leads to the same set of dimensionless variables with one exception. The jet momentum ratio J and the ratio of puncture diameter to river depth D/d for the continuous spill are replaced by r_i/d where r_i is the characteristic radius of the spill volume

$$V_i = \frac{4}{3} \pi r_i^3 \quad (IV.5)$$

IV.1.4 Experimental Test Plans

Experimental test plans were developed for both continuous and instantaneous spill model validation. A scale model ratio of $\lambda = 50$ was selected and a rectangular test channel with $w = 1.52m$ and $d = 0.24m$ was constructed at Texas A&M University for the laboratory scale experiments.

The original test plan for the continuous spill experiments is shown in Table IV.4. This plan was a 1/2 fractional factorial test matrix developed for

- o three levels of specific gravity
 - ethanol, 0.79
 - sucrose, 1.05
 - sodium silicate, 1.5
- o two values of densimetric Froude number

TABLE IV.4 ORIGINAL TEST PLAN FOR VALIDATION
OF THE CONTINUOUS SPILL MODEL

Run Number	ρ_c/ρ	J	Fr	u_*/u	θ_c
I.2 - 1	0.79	12.6	-.061	0.05	0°
I.2 - 2	0.79	202	-.061	0.05	90°
I.2 - 3	0.79	0.79	-.97	0.05	90°
I.2 - 4	0.79	12.6	-.97	0.05	0°
I.2 - 5	0.79	12.6	-.061	0.10	90°
I.2 - 6	0.79	202	-.061	0.10	0°
I.2 - 7	0.79	0.79	-.97	0.10	0°
I.2 - 8	0.79	12.6	-.97	0.10	90°
I.2 - 9	1.05	16.8	.26	0.05	0°
I.2 - 10	1.05	270	.26	0.05	90°
I.2 - 11	1.05	1.05	4.1	0.05	90°
I.2 - 12	1.05	16.8	4.1	0.05	0°
I.2 - 13	1.05	16.8	.26	0.10	90°
I.2 - 14	1.05	270	.26	0.10	0°
I.2 - 15	1.05	1.05	4.1	0.10	0°
I.2 - 16	1.05	16.8	4.1	0.10	90°
I.2 - 17	1.5	24	.026	0.05	0°
I.2 - 18	1.5	384	.026	0.05	90°
I.2 - 19	1.5	1.5	.41	0.05	90°
I.2 - 20	1.5	24	.41	0.05	0°
I.2 - 21	1.5	24	.026	0.10	90°
I.2 - 22	1.5	384	.026	0.10	0°
I.2 - 23	1.5	1.5	.41	0.10	0°
I.2 - 24	1.5	24	.41	0.10	90°

- o two values of jet momentum ratio
- o two values of friction velocity
 - $u_*/u = 0.05$
 - $u_*/u = 0.10$
- o two values of discharge angle, θ_c

Before the test program was begun it was believed that this set of tests, coupled with experimental measurements of buoyant plume trajectory performed earlier by S. J. Wright [19], would be ideal for the purpose of experimentally determining the plume entrainment parameters, α_1 , α_2 , and α_3 required by Ooms' VNF model. However, as the first tests were performed it became clear that the original test plan would have to be modified extensively. At the values of densimetric Froude number required by the test plan to simulate actual cargo spill conditions, plume buoyancy effects continued to influence the behavior of the chemical plume after the plume reached either the upper or lower channel surface. A set of concentration profile measurements was required that was more extensive than originally planned. Therefore, the test plan was modified and the experimental effort redirected as follows.

- o The sucrose solution with $Fr = 4.1$ showed an unexpectedly large amount of gravity spreading when the plume reached the channel floor. In order to validate the mixing and dilution model for cases of negligible buoyancy, a set of tests with dye mixed with water and $Fr = \infty$ was inserted into the test program.
- o Tests indicated that two levels of friction velocity for the turbulent channel flow could not be achieved without substantial modification (roughening) of the channel floor. Therefore, only tests with $u_*/u = 0.05$ were performed.
- o A sodium silicate solution with s.g. = 1.5 could not be produced. A more dilute sodium silicate solution with s.g. = 1.4 was substituted.
- o Chemical pool formation on the channel floor was found with the sodium silicate solution and a Froude number of 0.51. Tests at lower values of Fr (by reducing channel velocity) indicated that the pool would spread over the full width of the test channel.

A greater channel width would be needed if the pool were to reach its maximum equilibrium size. Therefore, all tests in the test plan with values of $Fr < 0.1$ had to be deleted from the test program.

- o Flow visualization tests with $\theta_c = 90^\circ$ (vertical downward) indicated that this discharge angle simply produced a quicker transition to the Colenbrander model. These tests were deleted in order to concentrate the maximum effort on the $\theta_c = 0^\circ$ cases that produced surface plume spreading due to buoyancy.

The final test plan for validation of the continuous spill model is shown in Table IV.5.

The test plan developed for validation of the instantaneous spill model was modified in a similar manner. The original test matrix is shown in Table IV.6. Tests with $u_*/u = 0.10$ were deleted while a set of tests with water and dye was inserted. The series of tests with $r_i/d = 0.5$ proved to be too large for the laboratory channel. However, tests with $r_i/d = 0.125$ and 0.23 were performed. The final test plan is shown in Table IV.7.

Although the number of tests included in the final test plan was smaller than in the original test plan, the amount of data acquired per test was more comprehensive. Cross-stream and depth-wise concentrations were measured at several downstream locations (or for several times) for each test. The test data was more than adequate to serve the purposes of model validation.

TABLE IV.5 FINAL TEST PLAN FOR VALIDATING THE
CONTINUOUS SPILL MODEL

Run Number	ρ_c/ρ	J	Fr	u_*/u	θ_c
I.2 - 3	0.79	0.79	-0.97	.05	0°
I.2 - 4	0.79	12.6	-0.97	.05	0°
I.2 - 9	1.05	16.8	0.26	.05	0°
I.2 - 11	1.05	1.05	4.1	.05	0°
I.2 - 12	1.05	16.8	4.1	.05	0°
I.2 - 19	1.40	1.4	0.51	.05	0°
I.2 - 20	1.40	22.4	0.51	.05	0°
I.2 - 26	1.0	16.0	Infinite	.05	0°
I.2 - 27	1.05	7.5	0.51	.05	0°

TABLE IV.6 ORIGINAL TEST PLAN FOR VALIDATION OF THE
INSTANTANEOUS SPILL MODEL

Run Number	ρ_c/ρ	r_i/d	u_*/u
II.1 - 1	0.79	0.125	0.05
II.1 - 2	0.79	0.25	0.05
II.1 - 3	0.79	0.50	0.05
II.1 - 4	0.79	0.125	0.10
II.1 - 5	0.79	0.25	0.10
II.1 - 6	0.79	0.50	0.10
II.1 - 7	1.05	0.125	0.05
II.1 - 8	1.05	0.25	0.05
II.1 - 9	1.05	0.50	0.05
II.1 - 10	1.05	0.125	0.10
II.1 - 11	1.05	0.25	0.10
II.1 - 12	1.05	0.50	0.10
II.1 - 13	1.50	0.125	0.05
II.1 - 14	1.50	0.25	0.05
II.1 - 15	1.50	0.50	0.05
II.1 - 16	1.50	0.125	0.10
II.1 - 17	1.50	0.25	0.10
II.1 - 18	1.50	0.50	0.10

TABLE IV.7 FINAL TEST PLAN FOR VERIFYING INSTANTANEOUS SPILL
MODEL PREDICTIONS

Run Number	ρ_c/ρ	Spill Material	r_i/d	V_i (cm ³)	u_*/u	u (cm/sec)
II.1 - 1	0.79	Ethyl Alcohol	0.125	103	0.05	14.1
II.1 - 2	0.79	"	0.23	904	0.05	14.1
II.1 - 7A	1.05	Sucrose	0.125	103	0.05	3.5
II.1 - 7B	1.05	"	0.125	103	0.05	14.1
II.1 - 8A	1.05	"	0.23	904	0.05	3.5
II.1 - 8B	1.05	"	0.23	904	0.05	14.1
II.1 - 13	1.40	Sodium Silicate	0.125	103	0.05	14.1
II.1 - 14	1.40	"	0.23	904	0.05	14.1
II.1 - 19	1.00	Water	0.125	103	0.05	14.1
II.1 - 20	1.00	"	0.23	904	0.05	14.1

IV.2 Data Collection Methodology

IV.2.1 Flow Channel

The 86' three-dimensional wave tank at Texas A&M University, College Station, Texas, was modified to provide the 50:1 scale model of a steady, non-tidal river specified in the test plan. The dimensions of this modified channel were 26.2m (86 ft) long, 152 cm (5 ft) wide, and 61 cm (2 ft) deep.

The water inlet area was constructed using a combination of a diffuser, baffles, weirs, rubberized hogs hair, and screens to yield a uniform flow field across the width of the channel. The spill location was 16 feet downstream of the last flow straightening screens. In the next 16-foot section, one wall was made of plexiglas for flow visualization purposes. Also in this area, stripes were painted on the floor, every two feet downstream and one foot cross-stream, and on the wall opposite the plexiglas wall, every two feet downstream and 2 inches vertically, to aid in quantifying results from flow visualization; an overall view of the channel is shown in Figure IV.3.

Water velocities ranged from 3.5 cm/sec to 14.1 cm/sec while maintaining a constant water depth of 24 cm (9-1/2 inches). The water velocities were controlled by valving of the supply water to the channel. The water depth was kept constant using an adjustable weir hinged on the channel floor. The channel floor roughness simulated a smooth channel with $u_*/u = 0.05$.

IV.2.2 Instrumentation

Detailed information about the horizontal and vertical velocity profiles and shear velocity was obtained using hot-film anemometry. The instrumentation used was a Thermo Systems, Inc. (TSI) Model 1051 Monitor & Power Supply coupled with a TSI Model 1050 Constant Temperature Anemometer equipped with a decade resistor. A TSI Model 1076 True RMS Voltmeter was used to obtain turbulence information necessary for calculation of the shear velocity. Six-mil hot-film probes were chosen to be appropriate for this

application and were mounted on a manually operated vertical and horizontal traversing mechanism.

Dye concentration measurements were obtained using a Turner Associates Model 430 Spectro-Fluorometer. In general, fluorometers measure the intensity of fluorescent light emitted by a sample under constant input light intensity. The measured intensity is directly proportional to the concentration of the fluorescent compound. This implies that, after calibration, dye concentrations can be read directly from the instrument.

Since the excitation and emission frequencies are different for various fluorescent dyes, appropriate filters must be used for each dye. The advantage of the Turner Associates Model 430 is that it is equipped with adjustable excitation and emission monochromators, similar to decade resistors, that allow more versatility than the colored glass filter fluorometers, also known as fluorimeters. The Model 430 also uses a Xenon light source as opposed to the UV light source of the fluorimeters.

IV.3 Data Collection

IV.3.1 Test Methods

Rhodamine WT, a fluorescent dye, was added to each spill chemical just before spilling. This was done so that when river samples were taken the fluorescence could be measured. The ratio of the local dye concentration, measured as fluorescence, to the dye concentration at the time of the spill yields the dilution of the dye and is thus the dilution of the spill chemical. Multiplication of this ratio by the spill density yields the local concentration. The dye was added to the chemical solutions in predetermined amounts so that the dye concentration in samples that had been diluted with water from the channel could be measured by the fluorometer.

For the continuous spills, the chemical and dye tracer mixture was discharged from a discharge port located at mid-water depth in the center of the channel width. The port was formed from a 1-cm-diameter tube bent 90° to give a discharge in the flow direction (0° is the angle

between the discharge direction and the river flow direction). An airfoil section was fitted to the downstream side of the discharge tube to minimize vortex formation and disturbances to the river velocity profile.

The spill setup for the continuous spills of chemical and dye is shown in Figure IV.3. The chemical and dye were premixed in the pictured can by a propeller attached to an electric motor. This mixture was then pumped to the port at the discharge rates specified in the test plan using a variable speed motor and a 1/4" rotary gear pump.

During discharge of the chemical and dye mixture, water samples from the channel were drawn through a sampling rake by a bank of ten peristaltic pumps and discharged into an array of sample bottles. Figures IV.4 and IV.5 show typical arrangements of the vertical and horizontal rakes, respectively. The spacing of the collection ports on the rakes were varied to maximize data collection over the height and width of the plume at the sampling location. Figure IV.6 shows the arrangement of the pumps and sample bottles above the sampling location.

The basic procedure was to take vertical $C(z)$ concentration profiles at three cross-stream (in the y-direction) locations for two or three downstream (in the x-direction) stations. The y, or cross-stream, locations were chosen from flow visualization to be in the center and within the left and right edges of the chemical and dye plume. The two x stations generally used were $x = 1.22m$ (48 in.) and $x = 3.05m$ (120 in.). The vertical center of the plume was located approximately from flow visualization, and a horizontal rake of equally spaced sample ports was set at the depth that corresponded to the maximum plume concentration.

To simulate "instantaneous" spills, the following procedure was used:

- o One end of an appropriately sized piece of PVC pipe was covered with a tightly stretched rubber bladder which was held by a hose clamp (see Figure IV.7).



FIGURE IV.3 SPILL SETUP FOR CONTINUOUS SPILLS

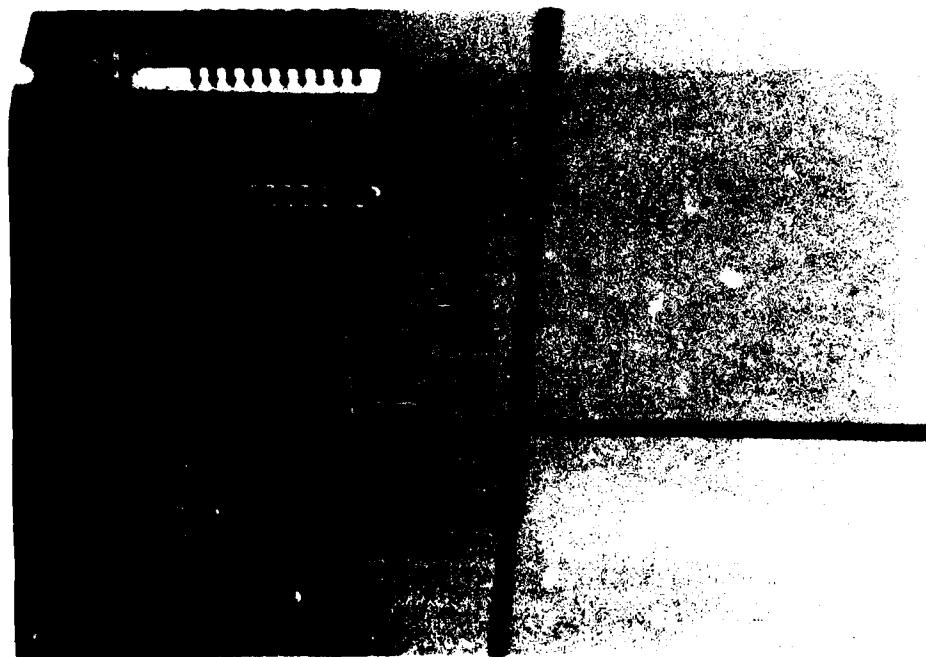


FIGURE IV.4 TYPICAL ARRANGEMENT OF THE VERTICAL RAKE ASSEMBLY

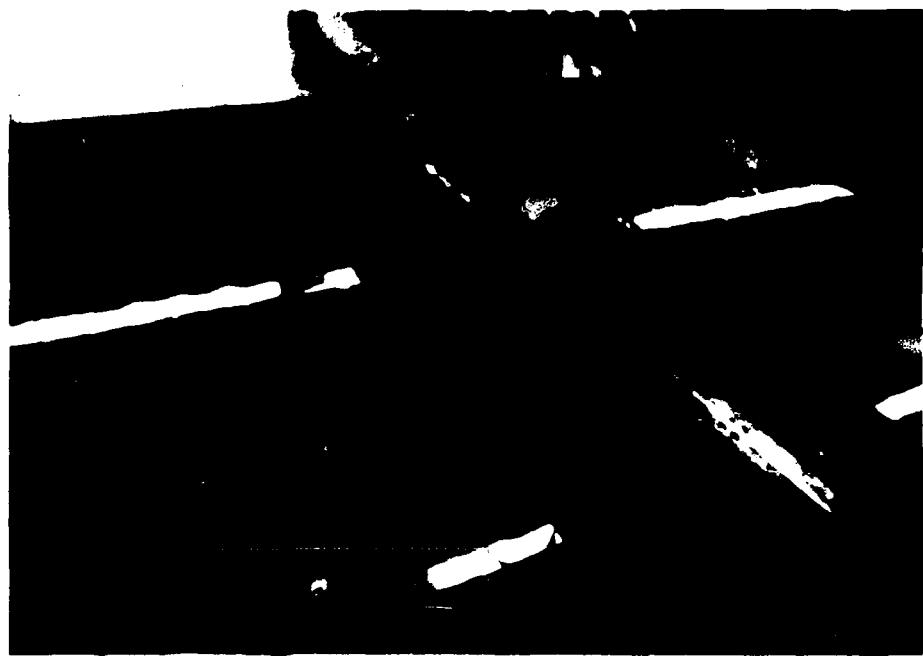


FIGURE IV.5 TYPICAL ARRANGEMENT OF THE HORIZONTAL RAKE ASSEMBLY

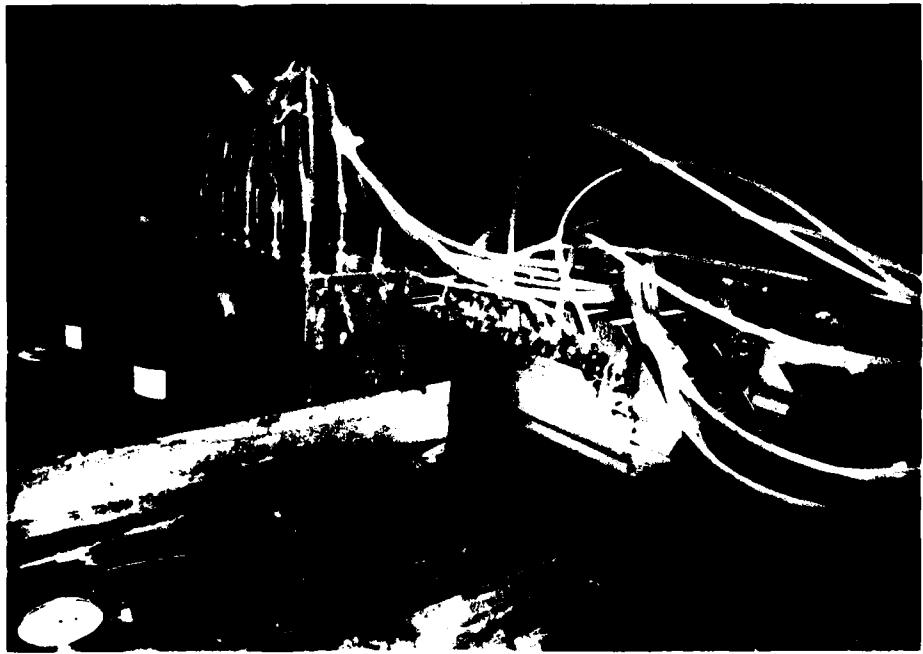


FIGURE IV.6 ARRANGEMENT OF THE SAMPLING PUMPS AND BOTTLES



FIGURE IV.7 INSTANTANEOUS SPILL CONTAINERS WITH TIGHTLY STRETCHED RUBBER BLADDER

- o The appropriate volume of chemical was poured into the open end of the PVC pipe and retained in the pipe by the bladder.
- o The PVC pipe was immersed into the water until the center of the column of chemical was at mid-depth of the water and centered in the channel; i.e., the center of the spill volume was placed at $x = 0$ in., $y = 0$ in., $z = 4.75$ inches.
- o From the top, with the aid of a razor blade attached to a rod, simultaneously the rubber bladder was broken and the pipe was lifted straight up and out of the water, releasing the chemical into the river. Figure IV.8 shows an alcohol spill soon after the spill was released.

To obtain river samples for analysis, a manually operated test tube rack was constructed so that fifteen sets of ten samples could be collected at various times as the spill passed by a certain x location downstream of the spill (Figure VI.9). The time between each set of collected samples depended on the spill material, spill size, and river speed. This time, based on flow visualization, was chosen to allow samples to be collected in 15 sets or less, over a large portion of the time it took for the spill to pass the designated x location. For the low river speed cases, the time for each sample set had to be increased to allow for collection of a large enough sample for analysis, since the sampling flow rate was specified so as to collect the samples isokinetically.

The sampling rake arrays were set up for each test at 4.27m (168 in.) downstream of the spill location, based on information gained during flow visualization. Figure IV.10 is a channel cross-sectional view of a typical sampling rake array with both a vertical and horizontal portion.

The vertical rake arrays were spaced and positioned based on the buoyancy of the chemical spilled. For neutrally buoyant spills, these rakes were spaced over the full depth of the water. For the positively

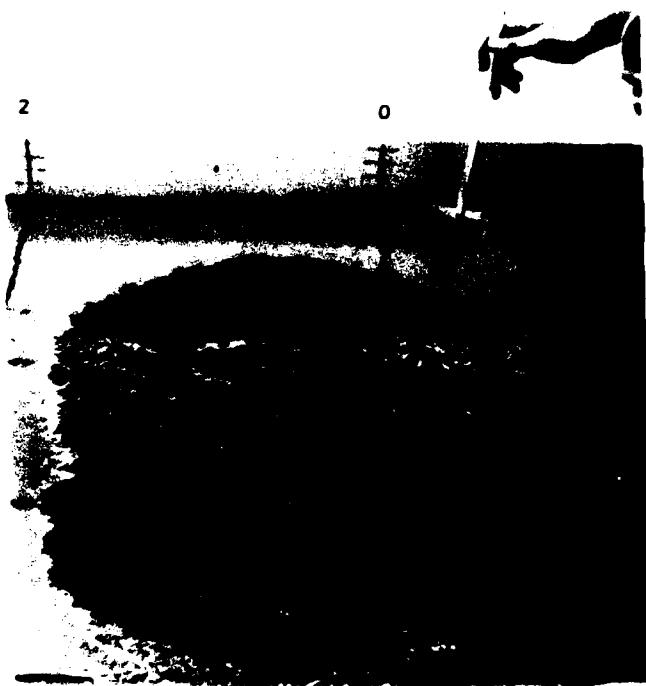


FIGURE IV.8 ETHYL ALCOHOL SPILL SOON AFTER AN INSTANTANEOUS RELEASE

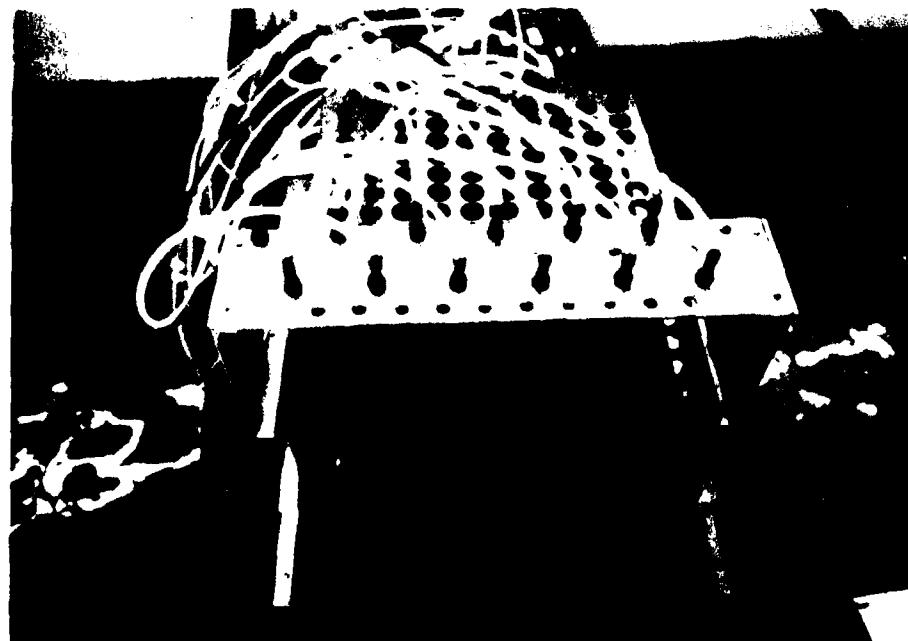


FIGURE IV.9 TEST TUBE RAKE FOR SAMPLING DURING INSTANTANEOUS SPILL TESTS

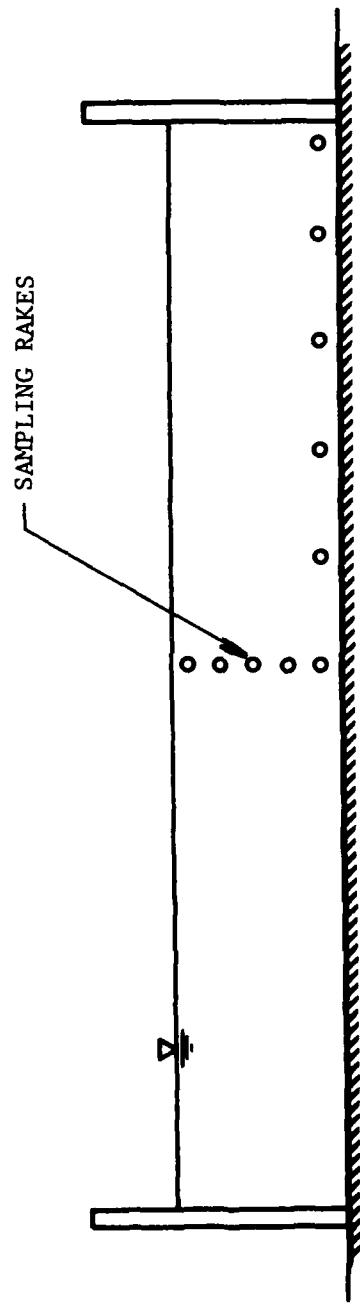


FIGURE IV.10 CHANNEL CROSS-SECTIONAL VIEW OF TYPICAL SAMPLING RAKE ARRAY

buoyant and negatively buoyant spills, the vertical rakes were spaced closer together and either raised to the free surface or lowered to the floor, respectively.

The depth of the horizontal rake arrays was also based on the buoyancy of the chemical spilled: near the free surface for the positively buoyant spills, near the center for neutrally buoyant spills, and near the floor for negatively buoyant spills.

Due to the desire to collect both vertical and horizontal concentration profile data during a single spill and the collection pump limitation of ten samples per set, the horizontal rake arrays spanned only one-half of the channel width. It is believed that the spills were symmetric about the channel centerline, and thus a concentration profile across the full width can be approximated by a reflection of the gathered data across this centerline.

IV.3.2 Test Results

The results of the hot-film anemometry velocity measurements for the two river velocities specified in the test plan are included as Figures IV.11 through IV.14. For each river velocity there is a graph of the horizontal velocity profile at $x = 3.05m$ (120 in.), showing that the flow field was fairly uniform across the channel width. There are also graphs of the vertical velocity profiles at $x = 3.05m$ (120 in.), showing that there was a turbulent boundary layer. Also indicated on the graphs of the vertical profiles are best-fit values of the shear velocity, u_* , for that river velocity. In both cases the ratio of shear velocity to free stream velocity is 0.04. This value is close to the 0.05 estimated in the test plan.

Only a general overview of the continuous spill experiments based on flow visualization will be presented in this section. For detailed information about each test, see Appendices K through S in the Test Data Volume of the Final Report. Included in these appendices are graphs of:

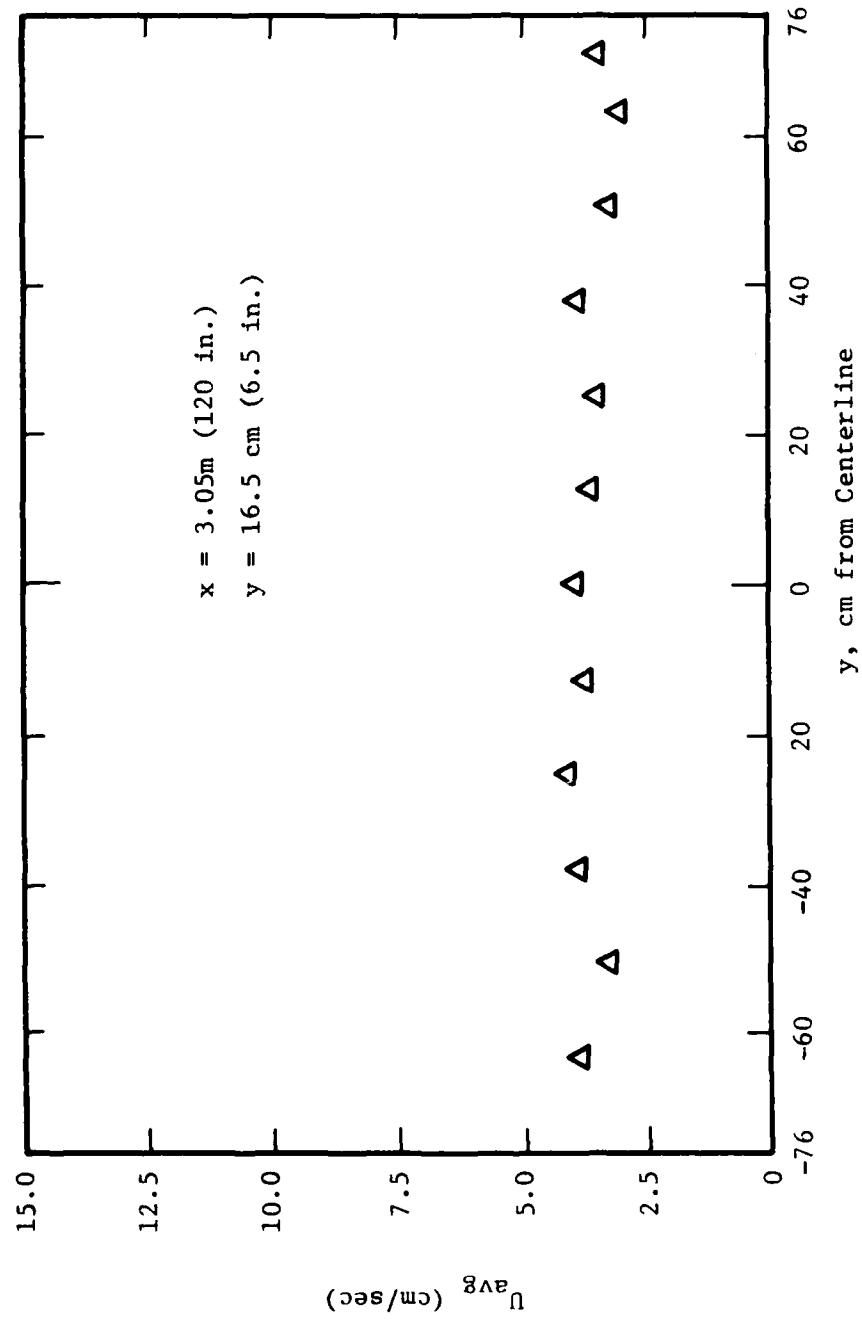


FIGURE IV.11 HORIZONTAL VELOCITY PROFILE FOR RIVER VELOCITY $\sim 3.5 \text{ cm/sec}$

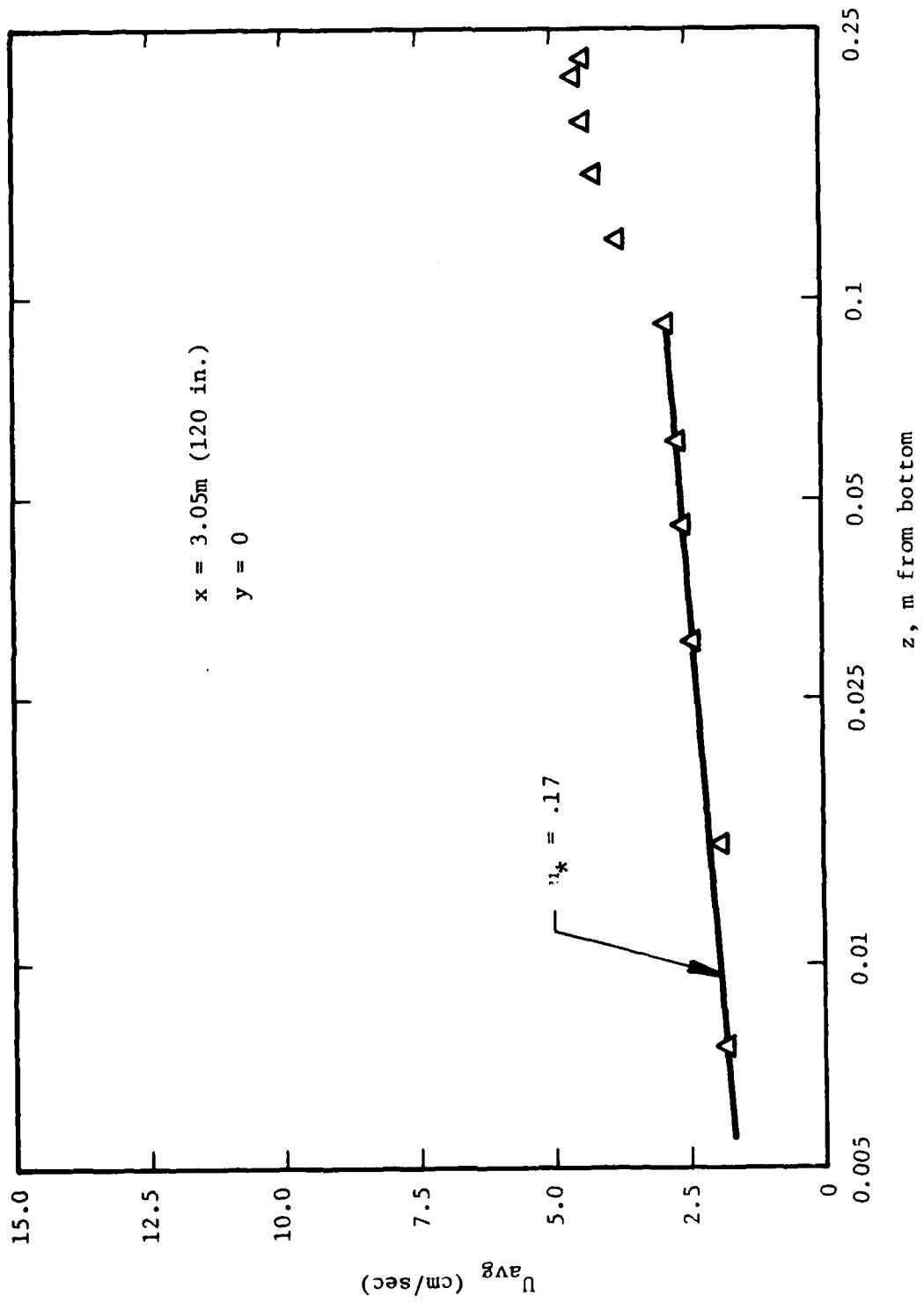


FIGURE IV.12 VERTICAL VELOCITY PROFILE FOR RIVER VELOCITY ≈ 3.5 cm/sec

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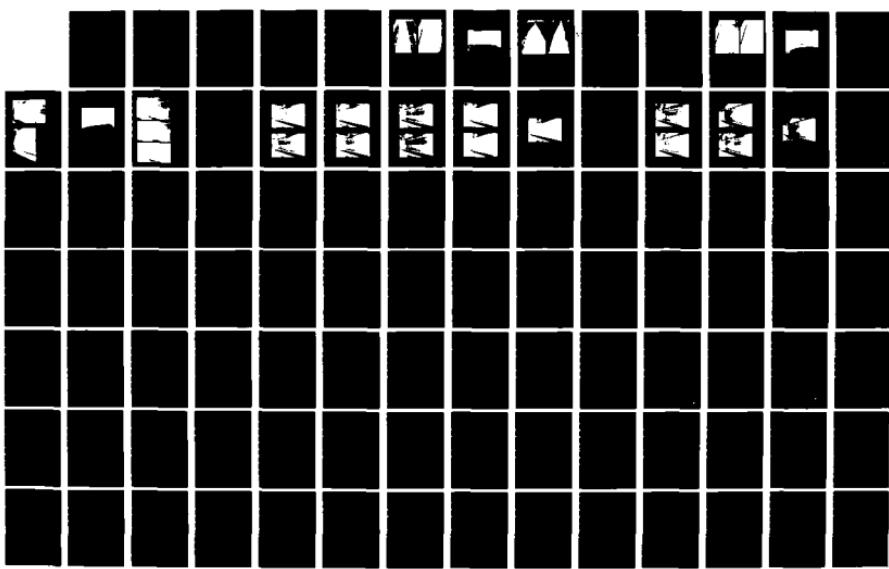
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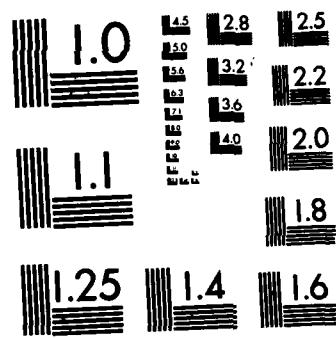
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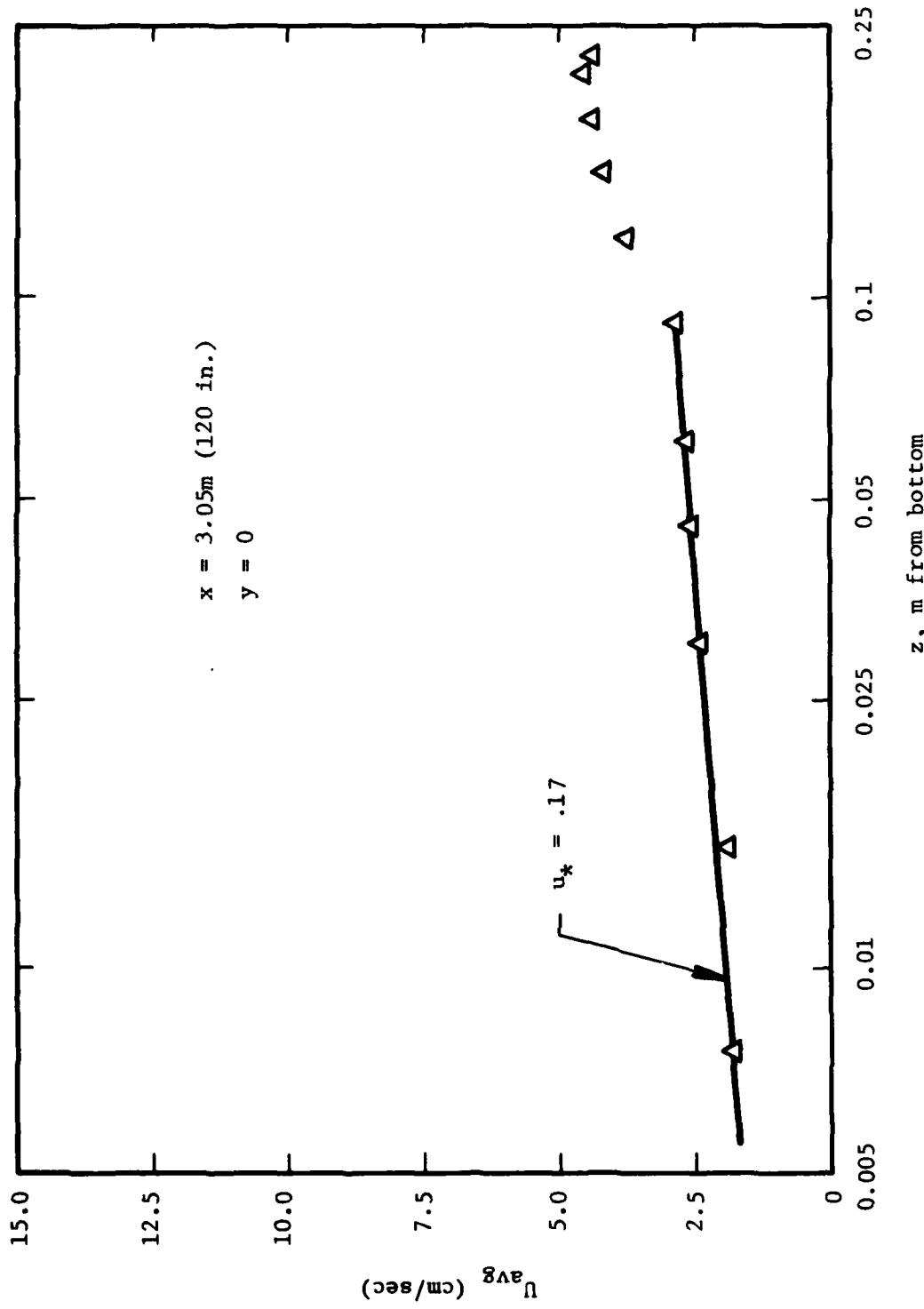


FIGURE IV.12 VERTICAL VELOCITY PROFILE FOR RIVER VELOCITY ≈ 3.5 cm/sec

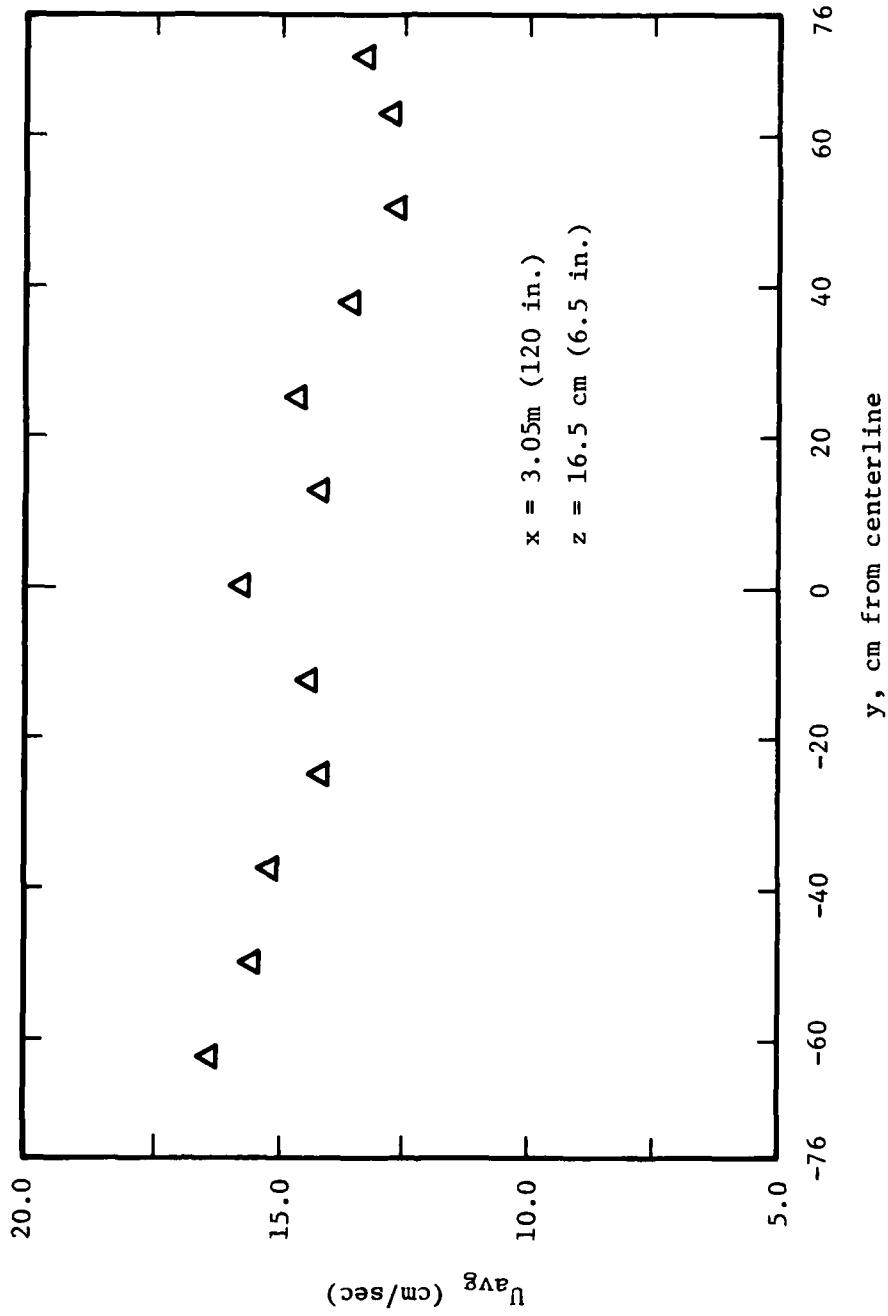


FIGURE IV.13 HORIZONTAL VELOCITY PROFILE FOR RIVER VELOCITY ≈ 14.1 cm/sec

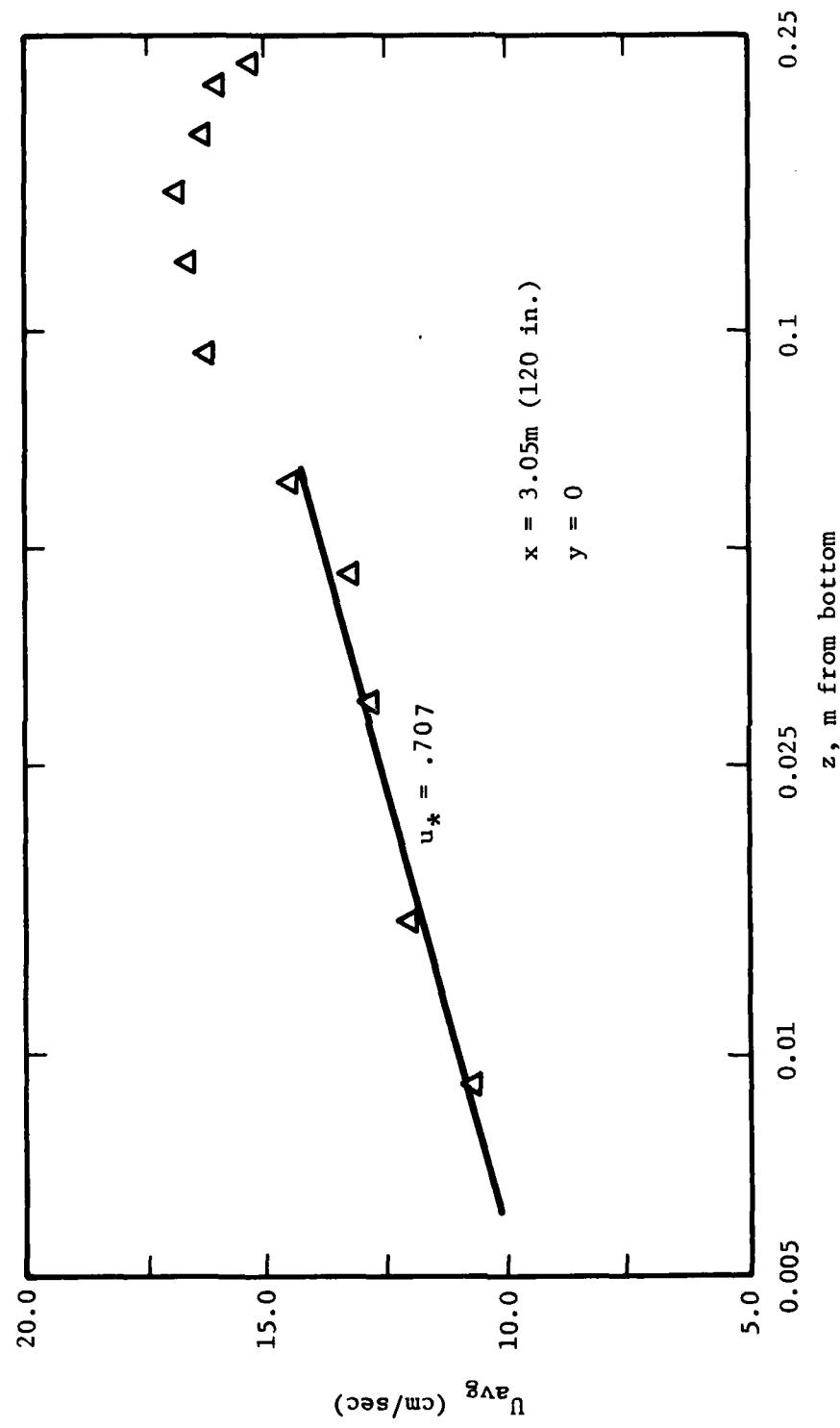


FIGURE IV.14 VERTICAL VELOCITY PROFILE FOR RIVER VELOCITY \approx 14.1 cm/sec

- (1) Cross-stream distance vs. concentration to aid in the understanding of the lateral mixing and dilution (y-direction).
- (2) Distance from free surface vs. concentration to aid in the understanding of the vertical mixing and dilution (z-direction).

Figure IV.15 shows photographs of the development of neutrally buoyant plumes of dye and water (specific gravity = 1.0) discharged at two different flow rates (44.4 and 11.1 cm^3/s) for the same river speed (14.1 cm/s). The dye plumes spread symmetrically in the vertical and lateral directions. The top and bottom edges of the dye plume reached the upper and lower river surfaces at a distance of about 183 cm (6 ft) downstream from the discharge port. The dye plume did not rise or fall after discharge, Figure IV.16, since the Froude number was infinite and buoyancy effects were absent.

Figure IV.17 shows a similar set of photographs of the development of negatively buoyant plumes of dye and sucrose (specific gravity = 1.05). The dye plumes fell vertically downward after discharge and hit the bottom of the channel at approximately 46 cm (18 in.) downstream of the discharge port. The dye plume then spread horizontally over the river bottom due to buoyant (gravity) effects. The amount of lateral spread at any downstream distance is greater at the higher discharge flowrate, condition A, than for the lower flowrate, condition B. The dye plume was concentrated in the lower 10 cm to 15 cm of the channel depth (total depth is about 24 cm). No dye was observed at the top of the channel within the first 488 cm (16 ft) downstream of the discharge port. Figures IV.18 and IV.19 are results for condition A, Run I.2-12, at 3.05m downstream. These are typical of the graphs included in the Test Data Volume.

Figure IV.20 shows a set of photographs of the development of positively buoyant plumes of dye and ethyl alcohol (specific gravity = 0.79). The dye plumes rose after discharge, as shown in Figure IV.21, and reached the upper channel surface at about 25 cm (12 in.) from the discharge port.



A



B

<u>Flow Conditions</u>	<u>River Speed</u>	<u>Discharge Flowrate</u>	<u>J</u>	<u>Fr</u>
A	14.1 cm/s	44.4 cm ³ /s	16.1	Infinite
B	14.1 cm/s	11.1 cm ³ /s	1.0	Infinite

FIGURE IV.15 FLOW VISUALIZATION OF CONTINUOUS DISCHARGE
OF A NEUTRALLY BUOYANT MIXTURE OF DYE AND WATER
(s.g. = 1.0)

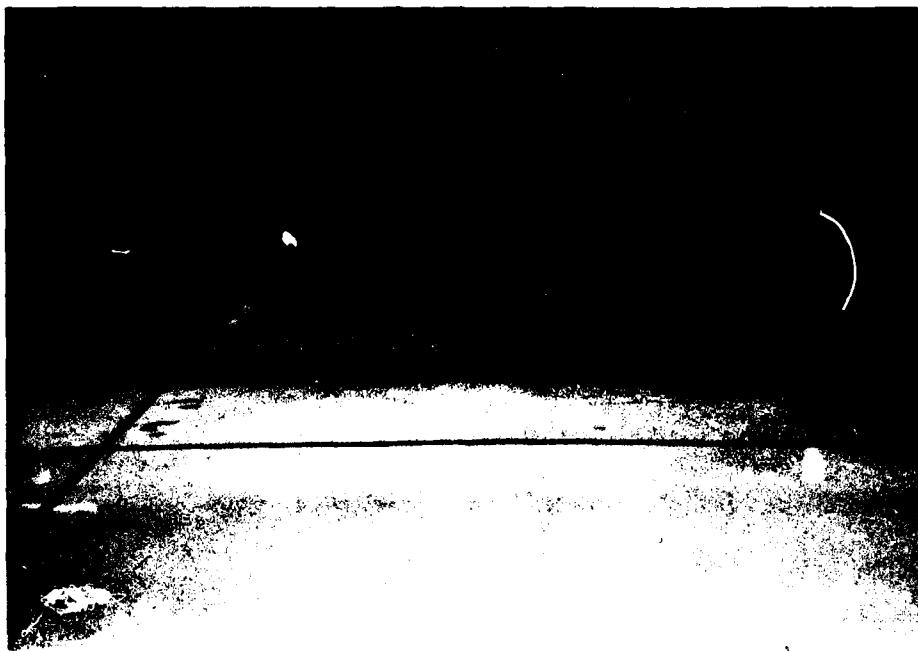
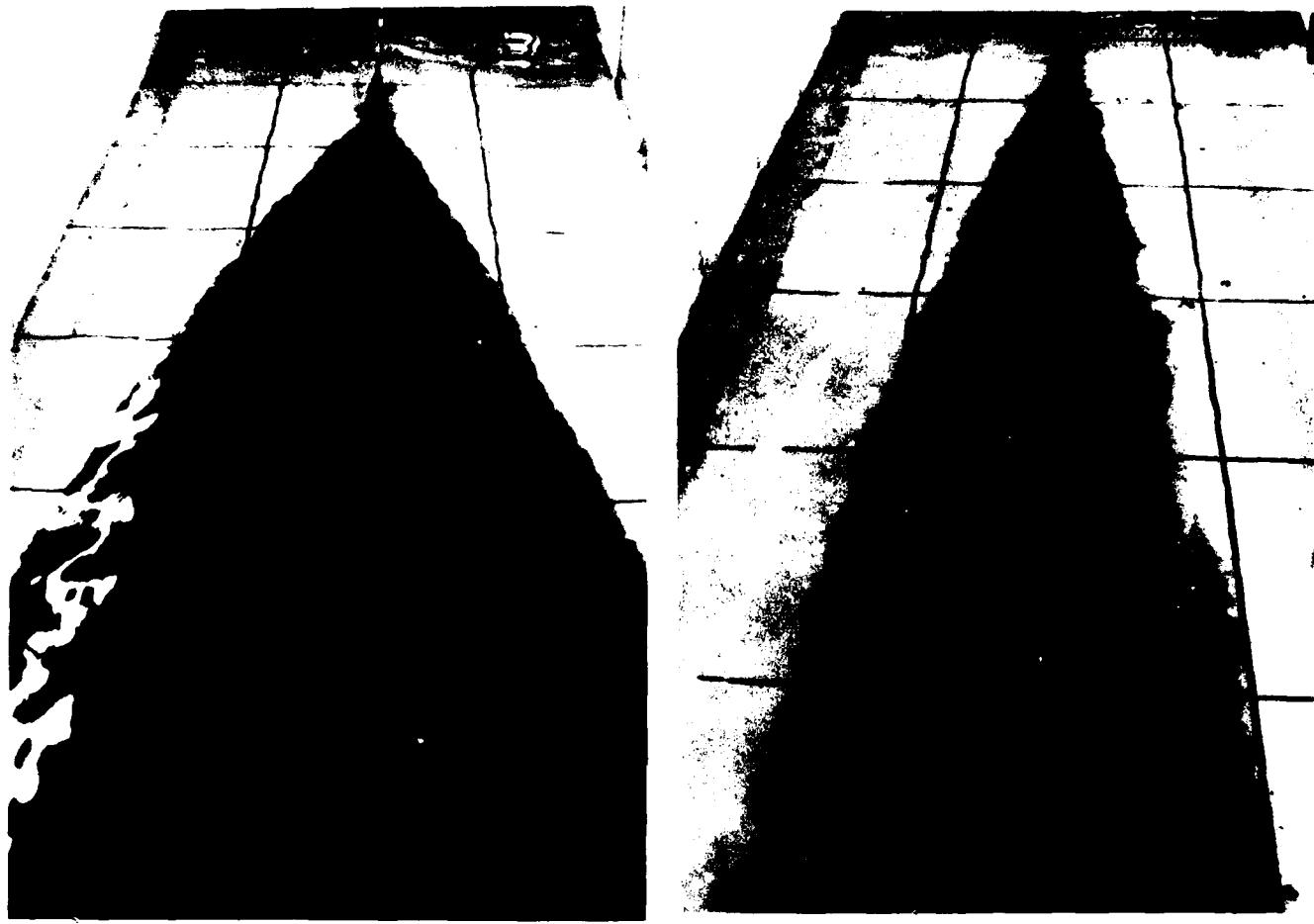


FIGURE IV.16 SIDE VIEW OF A NEUTRALLY BUOYANT PLUME



A

B

Flow Conditions	River Speed	Discharge Flowrate	J	Fr
A	14.1 cm/s	44.4 cm ³ /s	16.8	4.1
B	14.1 cm/s	11.1 cm ³ /s	1.05	4.1

FIGURE IV.17 FLOW VISUALIZATION OF CONTINUOUS DISCHARGE
OF A HEAVIER THAN WATER MIXTURE OF DYE AND SUCROSE
(s.g. = 1.05)

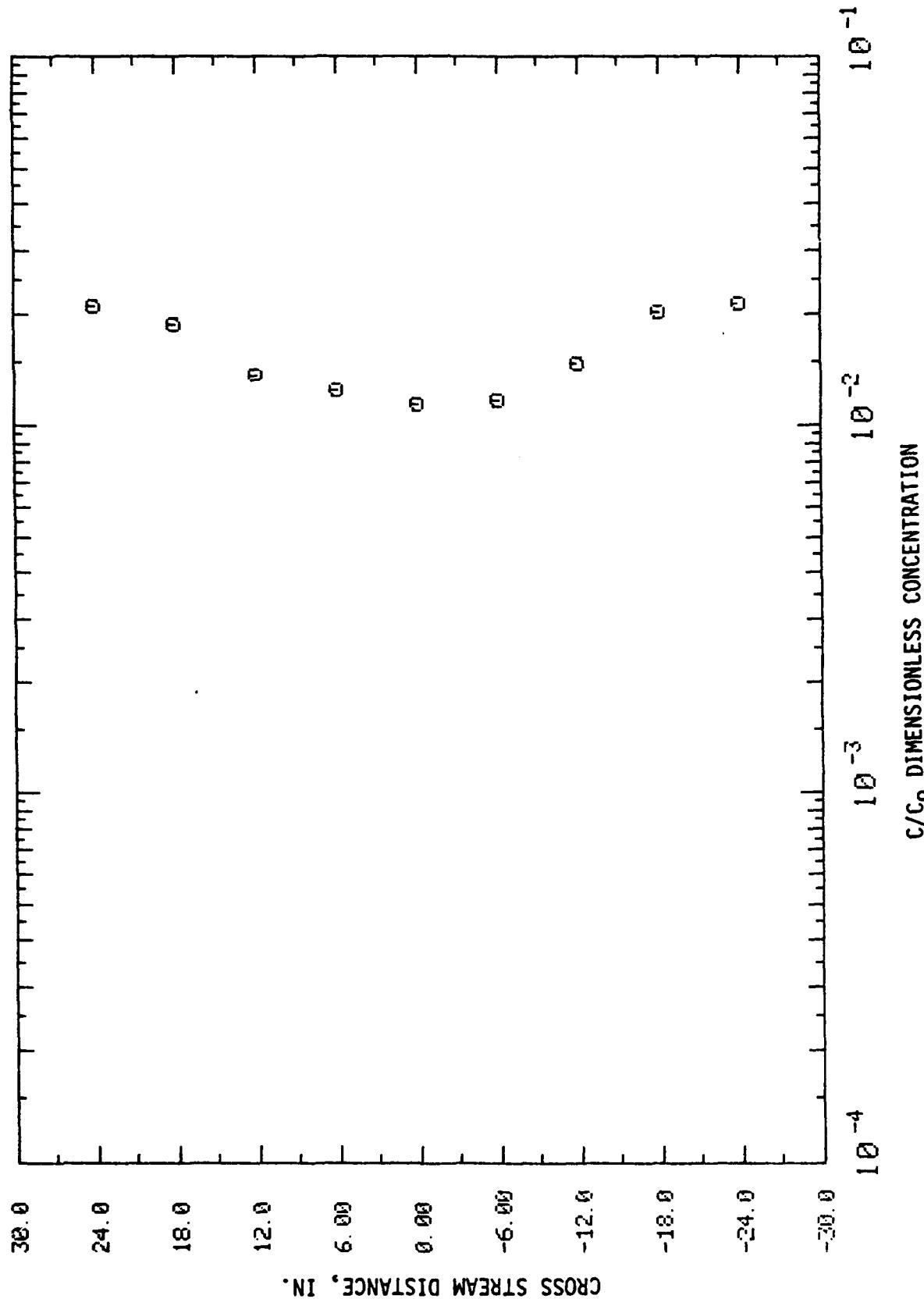


FIGURE IV.18 RUN 1.2-12 CROSS STREAM CONCENTRATION PROFILE

$x = 120$ IN., $z = 9.37$ IN.

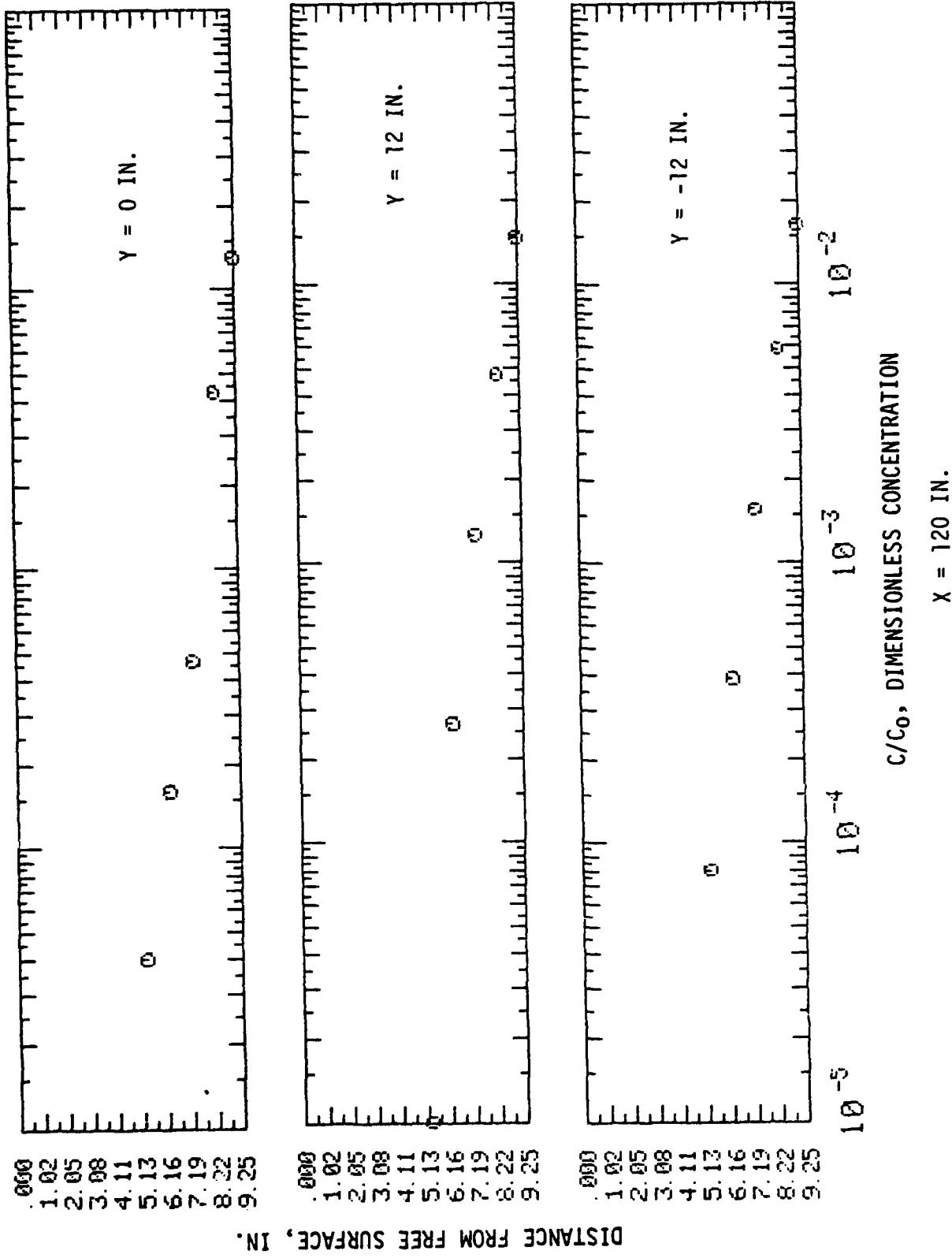
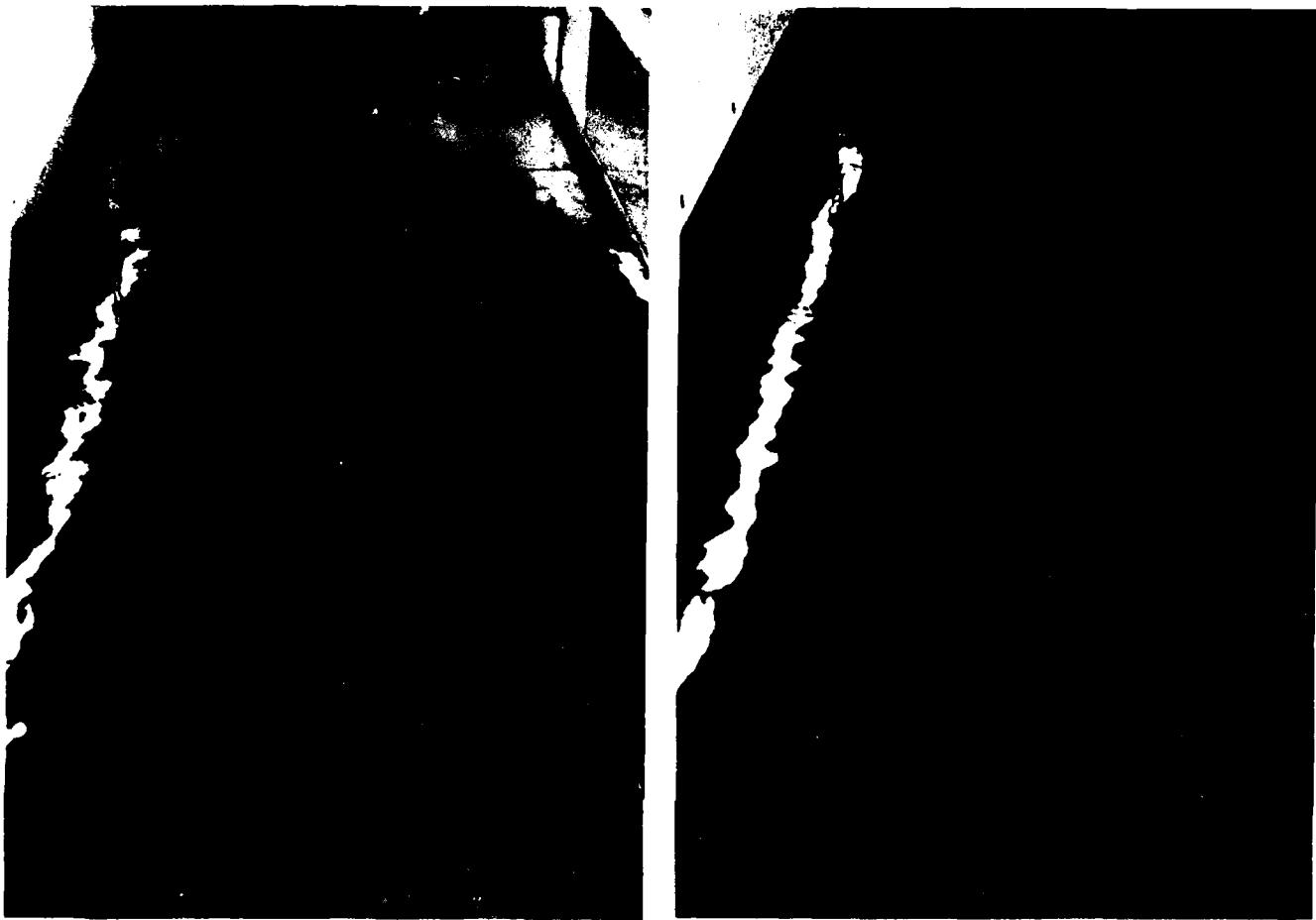


FIGURE IV.19 RUN I. 2-12 VERTICAL CONCENTRATION PROFILES



A

B

<u>Flow Conditions</u>	<u>River Speed</u>	<u>Discharge Flowrate</u>	<u>J</u>	<u>Fr</u>
A	14.1 cm/s	44.4 cm ³ /s	12.6	-0.97
B	14.1 cm/s	11.1 cm ³ /s	0.79	-0.97

FIGURE IV.20 FLOW VISUALIZATION OF CONTINUOUS DISCHARGE
OF A LIGHTER THAN WATER MIXTURE OF DYE AND
ETHYL ALCOHOL (s.g. = 0.79)

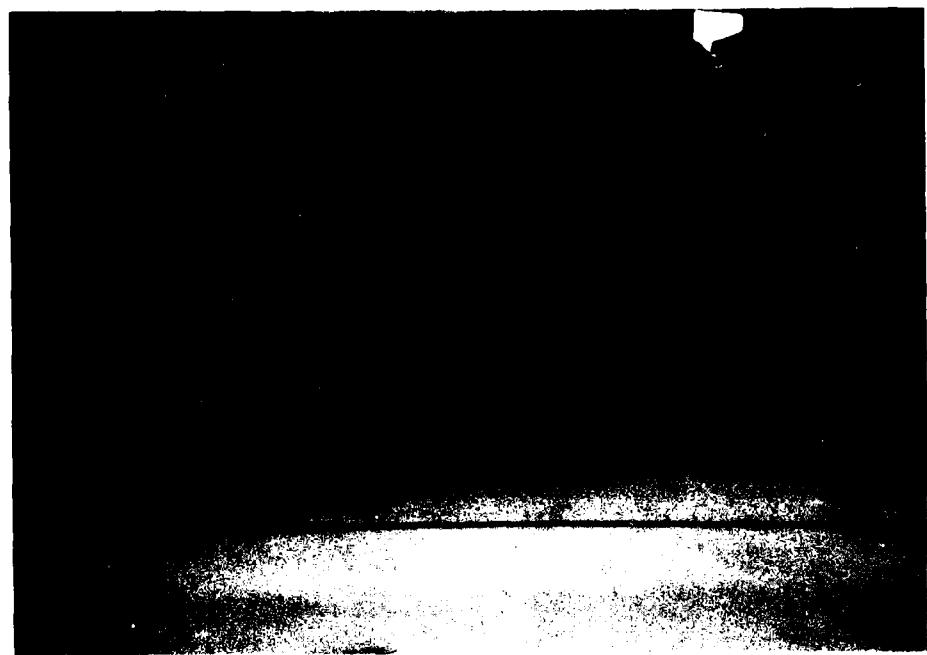


FIGURE IV.21 SIDE VIEW OF A POSITIVELY BUOYANT PLUME

The lateral buoyant spreading of the dye plume is noticeably more pronounced for the alcohol discharge than for the sucrose discharge in Figure IV.17. At the lower discharge flowrate, condition B, the dye plume was seen to bifurcate after hitting the water surface and spread downstream as two distinct dye plumes. The dye plume was concentrated in the upper 7 to 15 cm of the channel depth. No dye was observed at the bottom of the channel.

Figure IV.22 shows the set of photographs of the development of negatively buoyant plumes of dye and sodium silicate (specific gravity = 1.4). The dye plumes fell rapidly, Figure IV.23, after discharge and reached the bottom of the channel within 15 cm (6 in.) from the discharge port. The dye plumes spread laterally very rapidly with the same dependence on flowrate as seen in Figures IV.17 and IV.20. Figure IV.24 shows successive stages of the development of the sodium silicate plume with a flowrate of $44.4 \text{ cm}^3/\text{s}$. The dye plume had spread out over the full width of the channel (152 cm or 5 ft) by the time the leading edge reached a distance of 244 cm (8 ft) from the discharge port. The height of the dye plume was very small, only about 1 cm in thickness at a distance of 488 cm downstream from the discharge port.

As for the continuous spills, only a general overview of the instantaneous results based on flow visualization and review of the measured concentration data will be presented in this section. Detailed information about each case included in Appendices A through J of the Test Data Volume which consist of graphs of:

- (1) Concentration vs. time for one representative location in the flow to aid in the understanding of the mixing and dilution in the direction of the stream (x-direction).
- (2) Cross-stream distance vs. concentration to aid in the understanding of the lateral mixing and dilution (y-direction).
- (3) Distance from free surface vs. concentration to aid in the understanding of the vertical mixing and dilution (z-direction).



<u>Flow Conditions</u>	<u>River Speed</u>	<u>Discharge Flowrate</u>	$\frac{J}{J}$	$\frac{Fr}{Fr}$
A	14.1 cm/s	44.4 cm^3/s	22.5	0.51
B	14.1 cm/s	11.1 cm^3/s	1.4	0.51

FIGURE IV.22 FLOW VISUALIZATION OF A CONTINUOUS DISCHARGE OF A HEAVIER THAN WATER MIXTURE OF DYE AND SODIUM SILICATE (s.g. = 1.40)

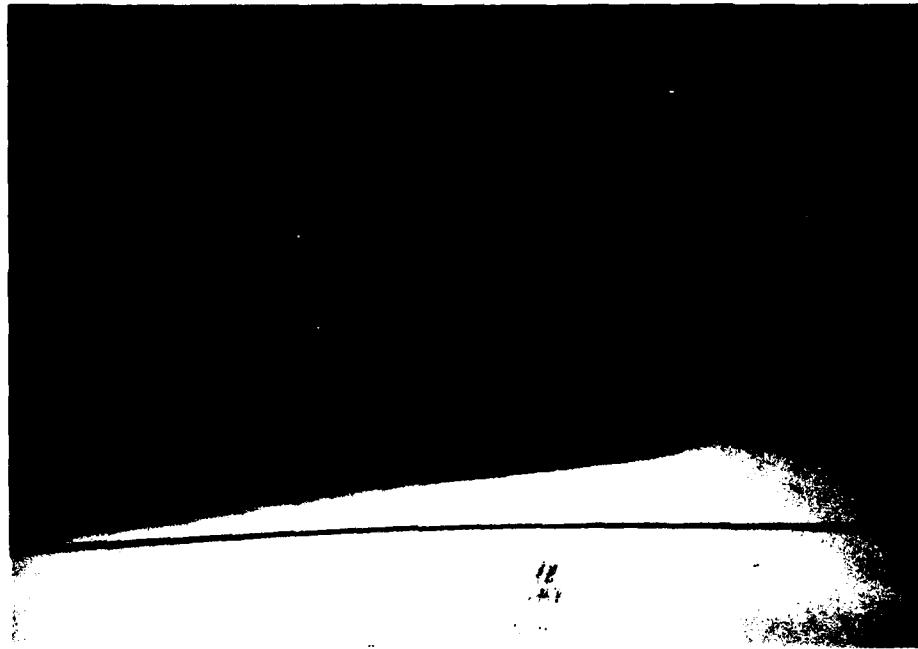
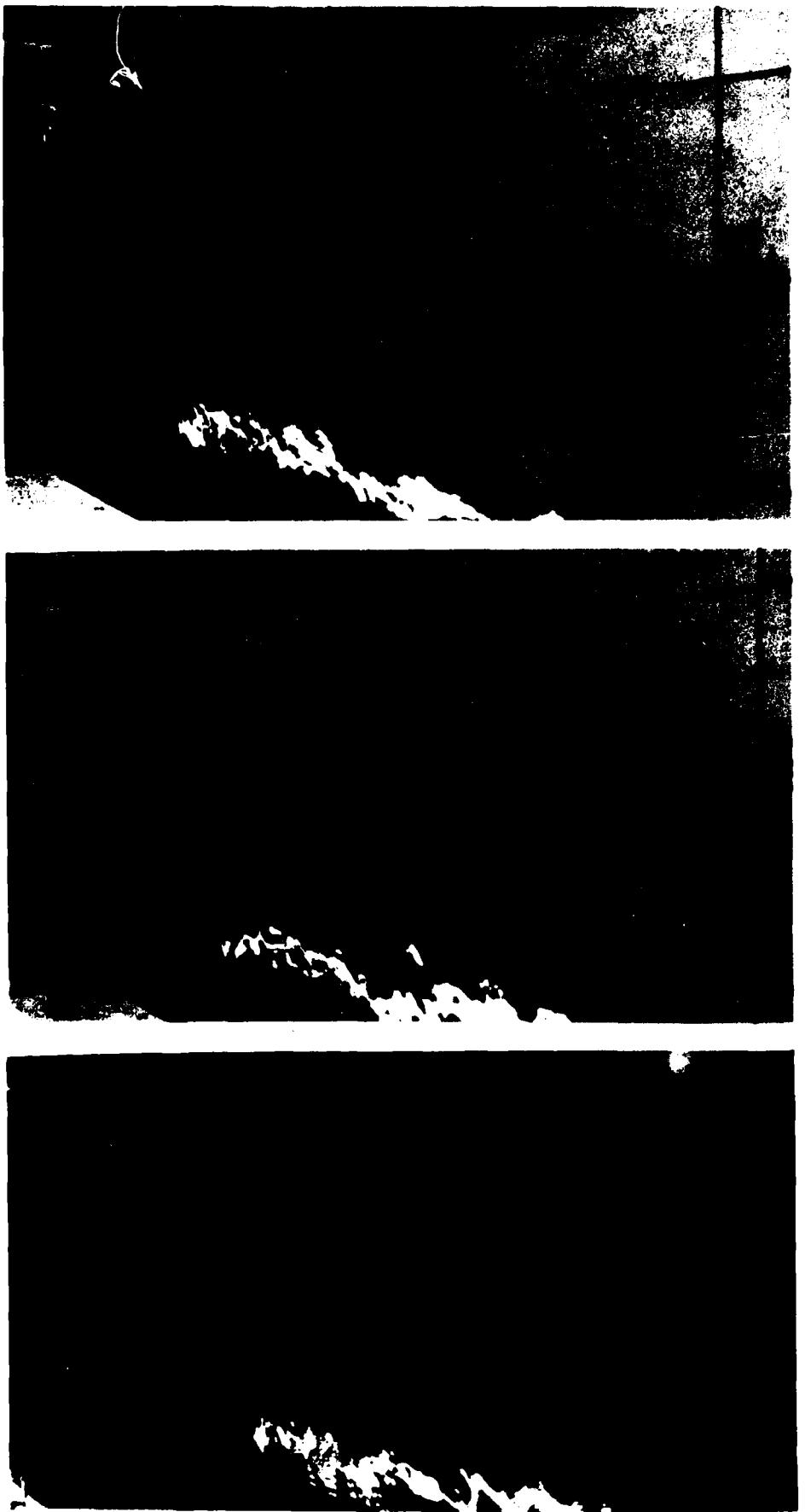


FIGURE IV.23 SIDE VIEW OF A NEGATIVELY BUOYANT PLUME



A11 correspond to Condition A of Figure 6.
A plume reaches 61 cm (2 ft). B plume reaches 122 cm (4 ft). C plume reaches 183 cm (6 ft)

FIGURE IV.24 FLOW VISUALIZATION OF THE DEVELOPMENT OF A CONTINUOUS DISCHARGE OF A HEAVIER THAN WATER MIXTURE OF DYE AND SODIUM SILICATE (s.g. = 1.40)

The series of photographs labeled Figure IV.25, shows a time lapse sequence of a 904 cm^3 instantaneous spill of a positively buoyant mixture of dye and ethyl alcohol (specific gravity = 0.79), specified in the test plan as Run II.1-2. As can be seen in this set of photographs, the chemical rose to the water surface and spread as a pool, quickly reaching the sides of the channel. The chemical was confined to within the top 6.35 cm of the river, even 4.27m (168 in.) downstream of the spill location. The 103 cm^3 spill of dye and ethyl alcohol (not shown) exhibited these same characteristics except that the chemical was confined to the top 5.0 cm of the river, 4.27 cm downstream of the spill.

The series of photographs labeled Figure IV.26, show a time lapse sequence of a 904 cm^3 instantaneous spill of a negatively buoyant mixture of dye and sodium silicate (specific gravity = 1.4), specified in the test plan as Run II.1-14. As can be seen, the chemical sank to the bottom of the channel and spread as a pool quickly reaching the sides of the channel. The chemical was confined to the lower 4.0 cm of the channel, even at 4.27m although the highest concentration was in the lower 1.5 cm of the channel. Also noticed in these photographs are the waves of chemical reflecting off the walls and moving back across the channel.

The 103 cm^3 instantaneous spill of dye and sodium silicate, Run II.1-13, exhibited slightly different characteristics. Due to the spill volume being smaller, the spill width at 4.27m downstream was measured to be only 61 cm (24 in.) in the 152 cm wide channel. Since the chemical had not yet reflected off the walls, the chemical was spread on the bottom slightly thinner than the 4.0 cm noted for the 904 cm^3 spill.

The instantaneous spills of negatively buoyant dye and sucrose (specific gravity = 1.05) exhibited many of the same characteristics as the 103 cm^3 dye and sodium silicate spill. The sucrose spills sank to the bottom of the channel but by 4.27m downstream had mixed more in the vertical direction and spread less in the horizontal direction. In some cases the spill was spread throughout the entire depth by this point.

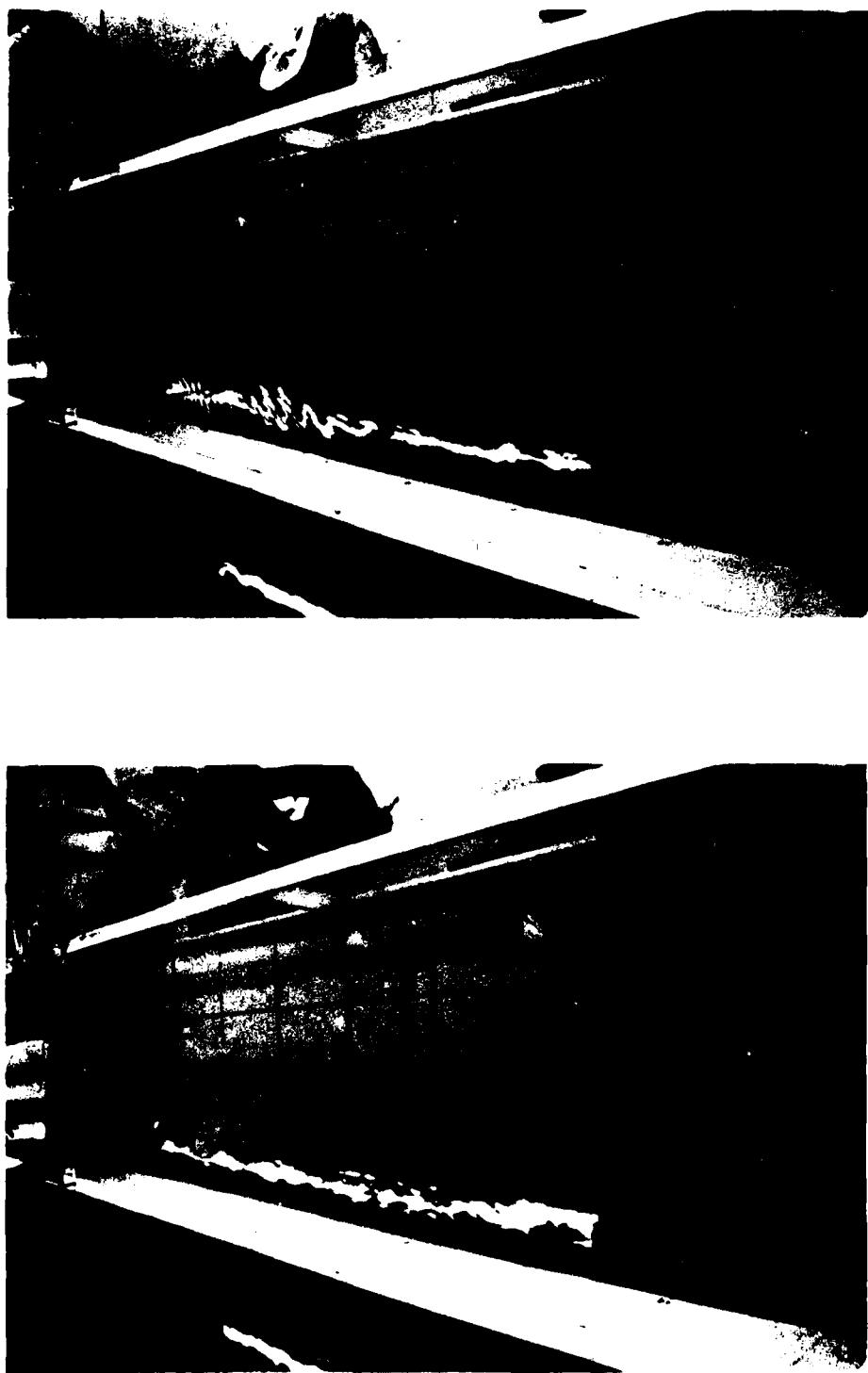


FIGURE IV.25 TIME LAPSE SEQUENCE OF AN INSTANTANEOUS SPILL OF ETHYL ALCOHOL AND DYE

FIGURE IV.25 TIME LAPSE SEQUENCE OF AN INSTANTANEOUS SPILL OF ETHYL ALCOHOL AND DYE (Contd)

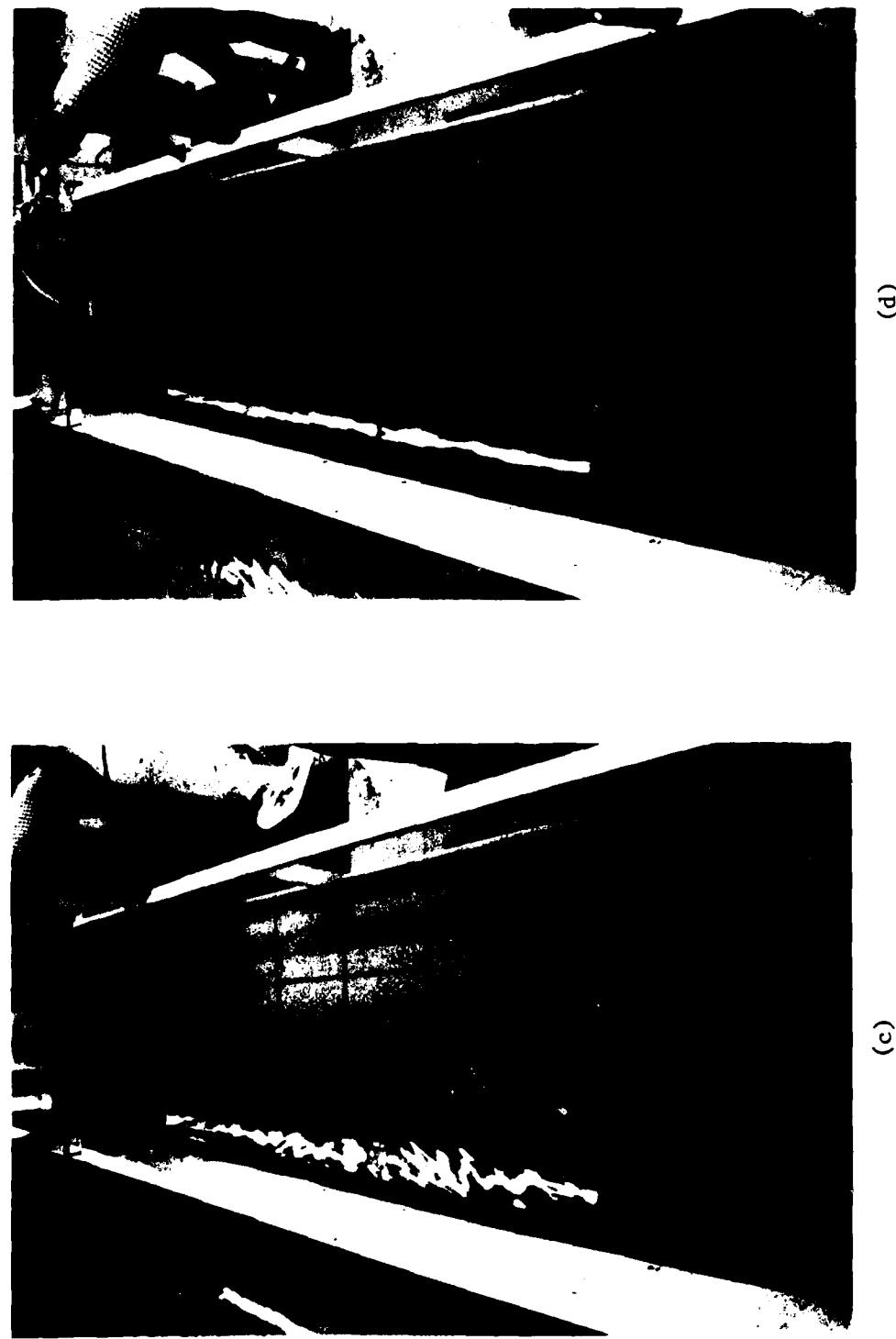


FIGURE IV.26 TIME LAPSE SEQUENCE OF AN INSTANTANEOUS SPILL OF SODIUM SILICATE AND DYE

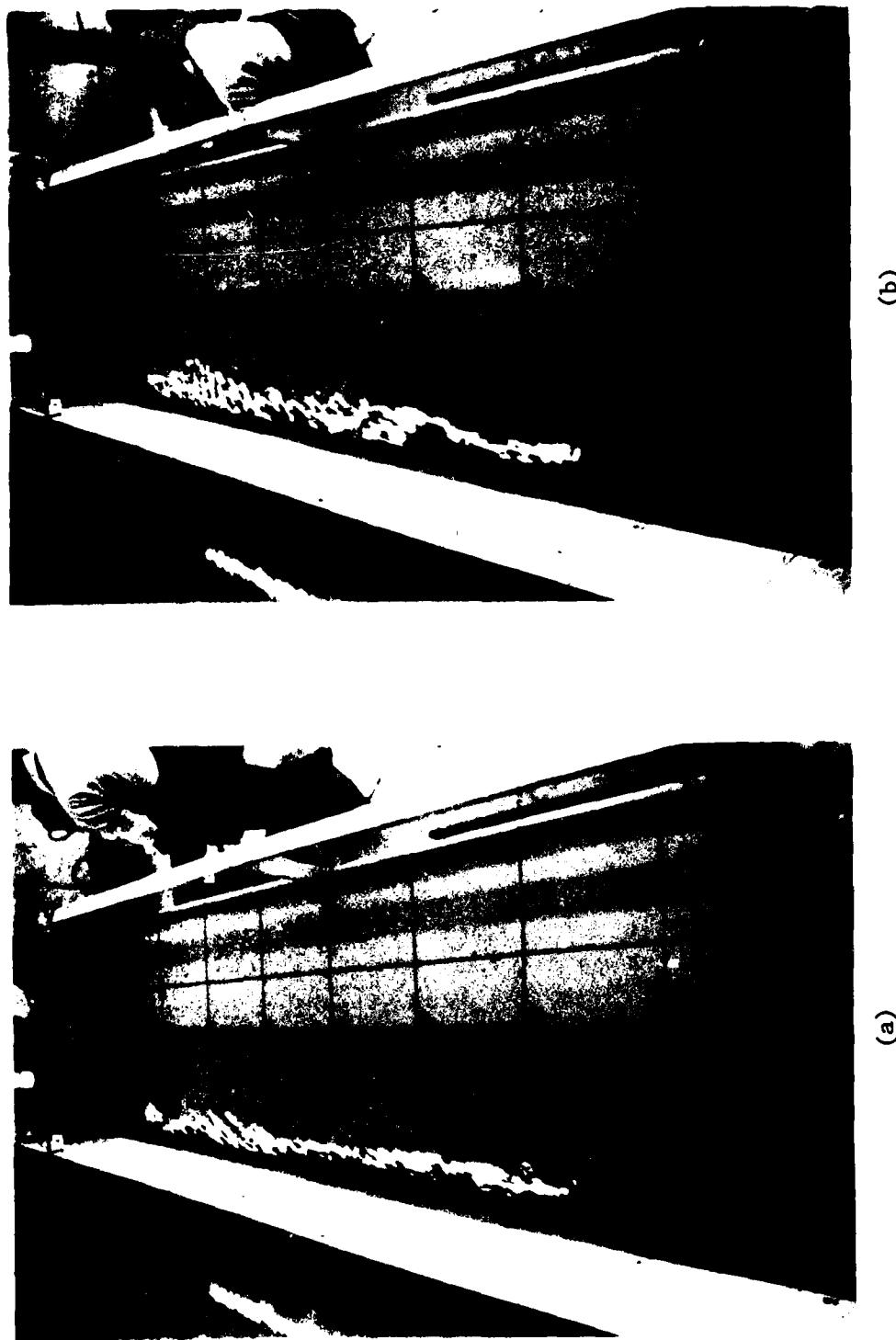
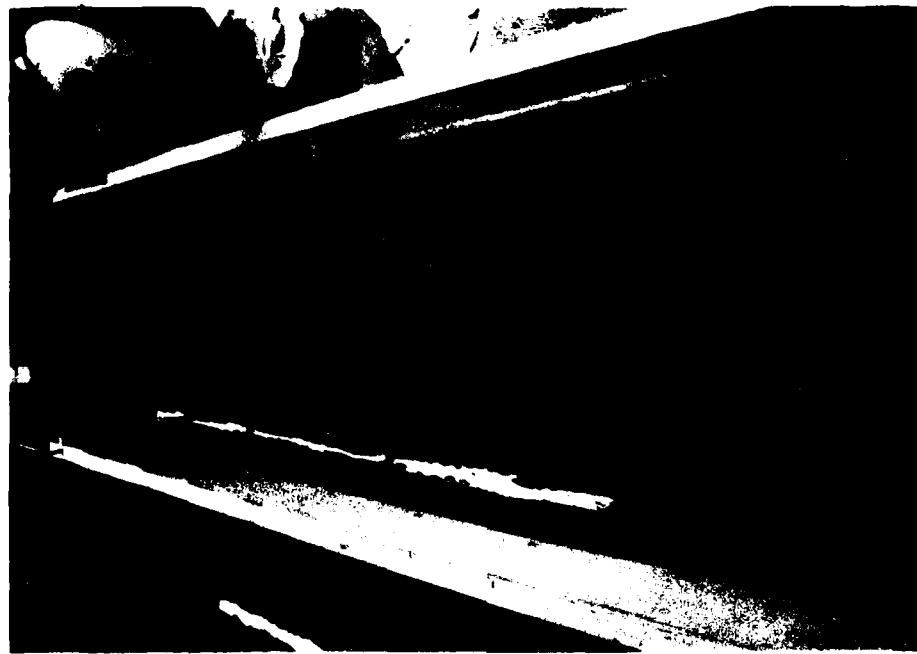


FIGURE IV.26 TIME LAPSE SEQUENCE OF AN INSTANTANEOUS SPILL OF SODIUM SILICATE AND DYE (Contd)

(c) (d)





(e)

FIGURE IV.26 TIME LAPSE SEQUENCE OF AN INSTANTANEOUS SPILL OF SODIUM SILICATE AND DYE (Contd)

The series of photographs labeled Figure IV.27, show a time lapse sequence of a 904 cm^3 instantaneous spill of a neutrally buoyant mixture of dye and water (specific gravity = 1.0), specified in the test plan at Run II.1-20. As can be seen, the spill stayed centered in the channel and dispersed vertically as well as laterally as it travelled down the channel. This spill spread to a width of less than 61.0 cm at the observation point 4.27m downstream of the spill location.

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(a)



(b)

FIGURE IV.27 TIME LAPSE SEQUENCE OF AN INSTANTANEOUS SPILL OF WATER AND DYE

FIGURE IV.27 TIME LAPSE SEQUENCE OF AN INSTANTANEOUS SPILL OF WATER AND DYE (Contd)

(d)



(c)

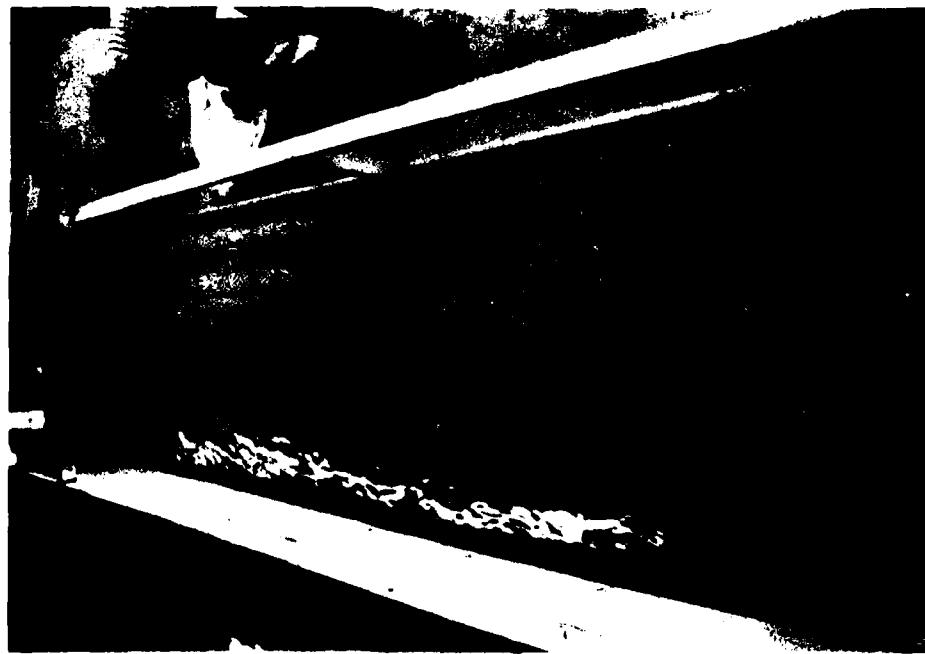


FIGURE IV.27 TIME LAPSE SEQUENCE OF AN INSTANTANEOUS SPILL OF WATER AND DYE (Contd)

(e)



V. COMPARISONS OF MODELS AND TESTS

As discussed in the preceding section, tests of continuous and instantaneous spills in a model steady river represent the data base for model verification. Since all the models contain one or more empirical constants, some of the test data were used to determine "best" values of the constants and other, independent tests were used to serve as comparisons to the model predictions.

V.1 Continuous Spills in Steady Rivers

This section presents a comparison of plume model predictions for plume width and concentration distribution with some of the data taken during the laboratory test program. For this comparison, one run was selected for each value of chemical specific gravity, 0.79, 1.0, 1.05, and 1.40. Model predictions were made using the same values of entrainment parameters for each run. Data from the runs with s.g. = 1.05 and 1.40 were used to derive a modified version of Colenbrander's $\phi(Ri_*)$ function (see Equation III.22). The modified function is

$$\phi(Ri_*) = 0.62 + 1.3911 \times Ri_*^{0.7} \quad (V.1)$$

In general, the agreement between plume model predictions and data is good. However, further optimization of the empirical parameters in both Ooms' and Colenbrander's models might improve the agreement even more.

Figures V.1 to V.4 compare model predictions with data for Run I.2-25, a continuous discharge of neutrally buoyant water and dye with s.g. = 1.0. Since this chemical has negligible buoyancy flux, its trajectory and dilution are sensitive only to the values of α_1 and α_3 , the entrainment coefficients for shear and channel turbulence. Figures V.1 and V.3 show that the cross-stream width of the plume is slightly overpredicted and the maximum concentration underpredicted at $x = 1.21m$ (48 inches) and $3.04m$ (120 inches). Likewise, the predicted vertical concentration profiles shown in Figures V.2 and V.4 are slightly "flatter" than indicated by the data. We may

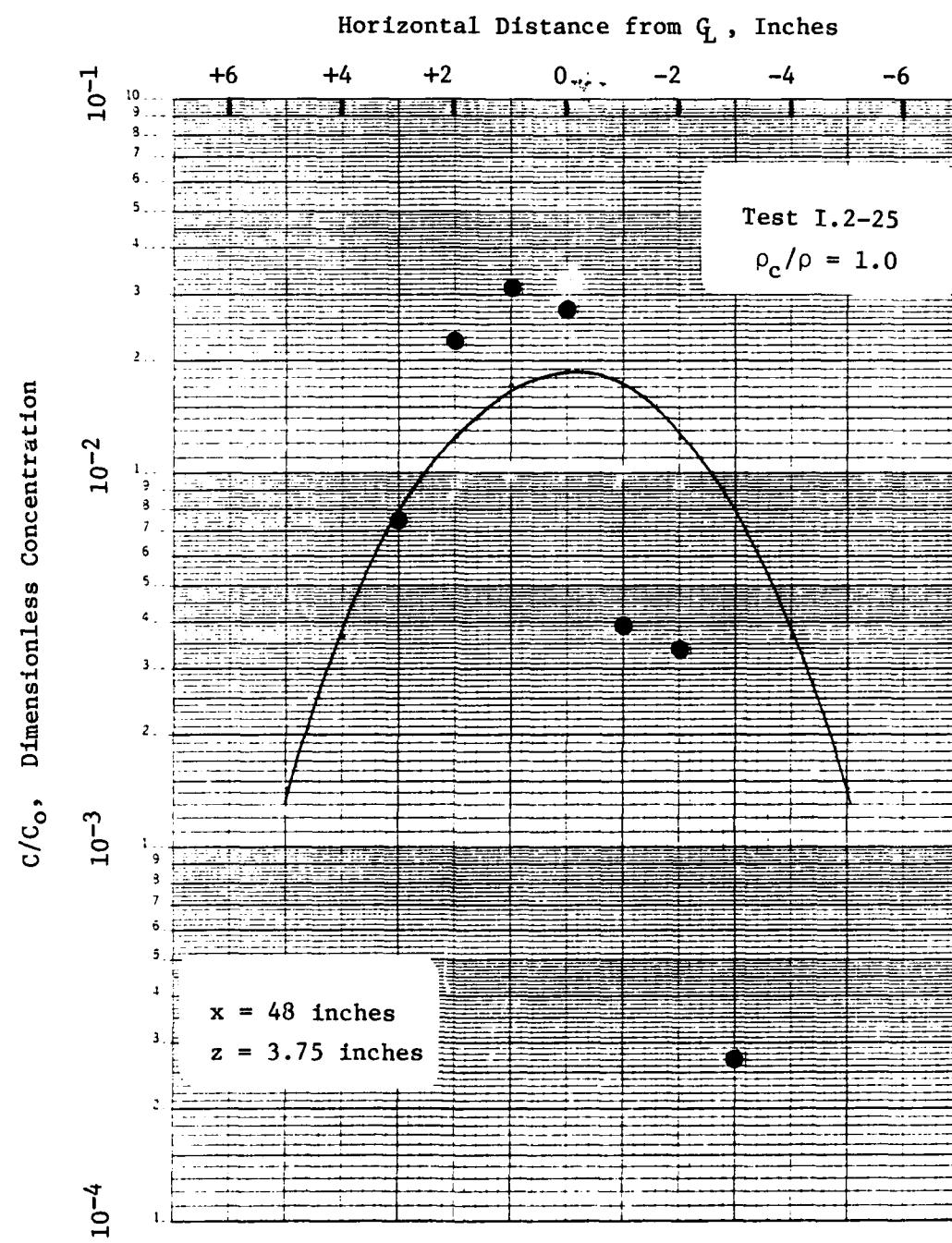
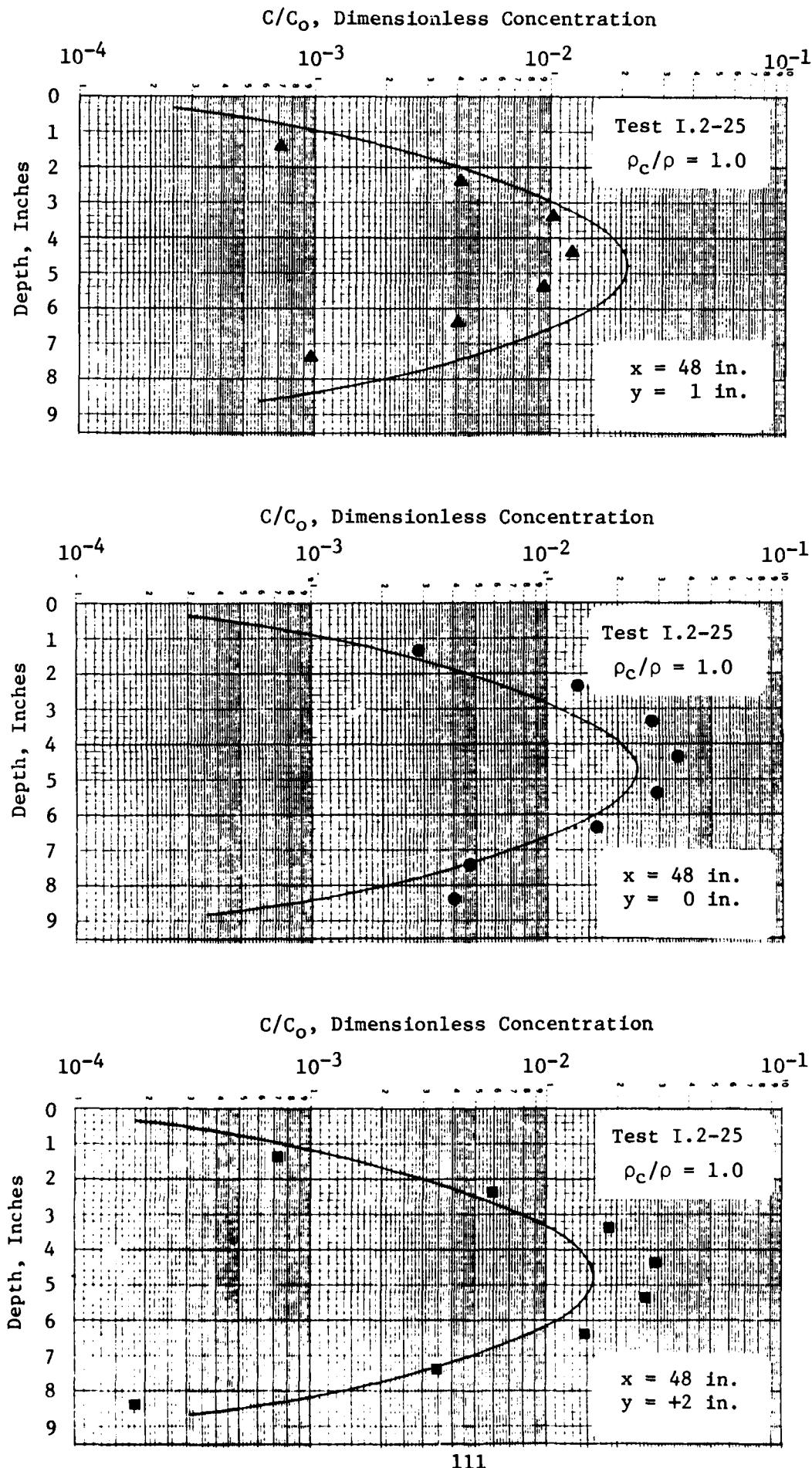


FIGURE V.1 CROSS-STREAM CONCENTRATION PROFILE
FOR CONTINUOUS SPILL OF NEUTRALLY BUOYANT
CHEMICAL

FIGURE V.2 VERTICAL CONCENTRATION PROFILES FOR CONTINUOUS SPILL
OF NEUTRALLY BUOYANT CHEMICAL



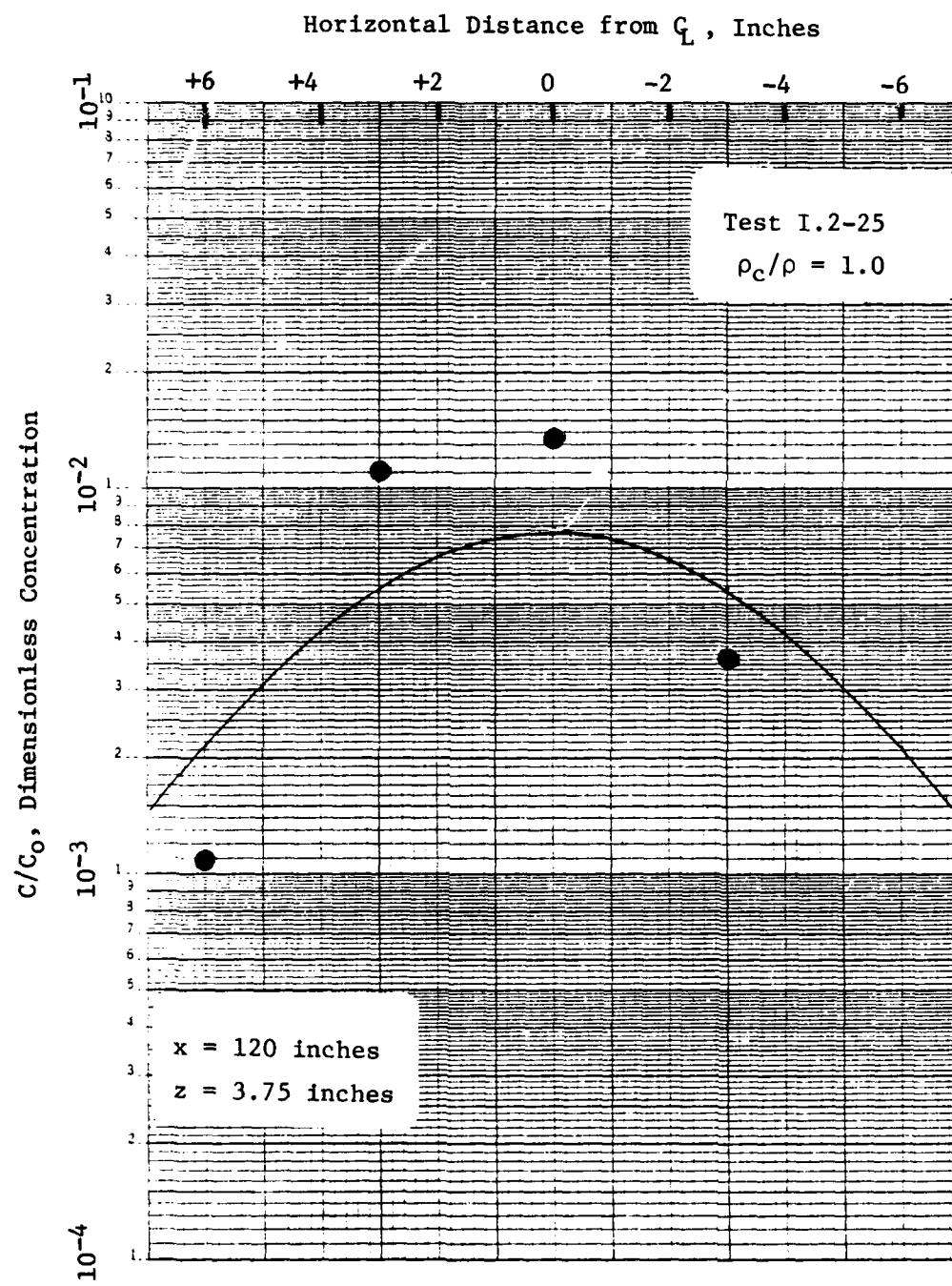


FIGURE V.3 CROSS-STREAM CONCENTRATION PROFILE
FOR CONTINUOUS SPILL OF NEUTRALLY BUOYANT
CHEMICAL

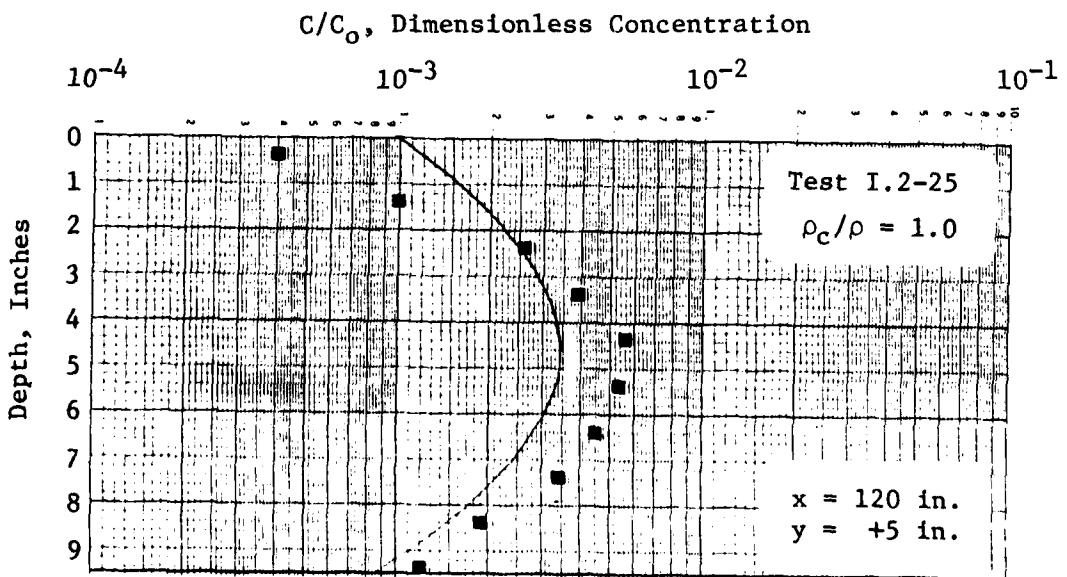
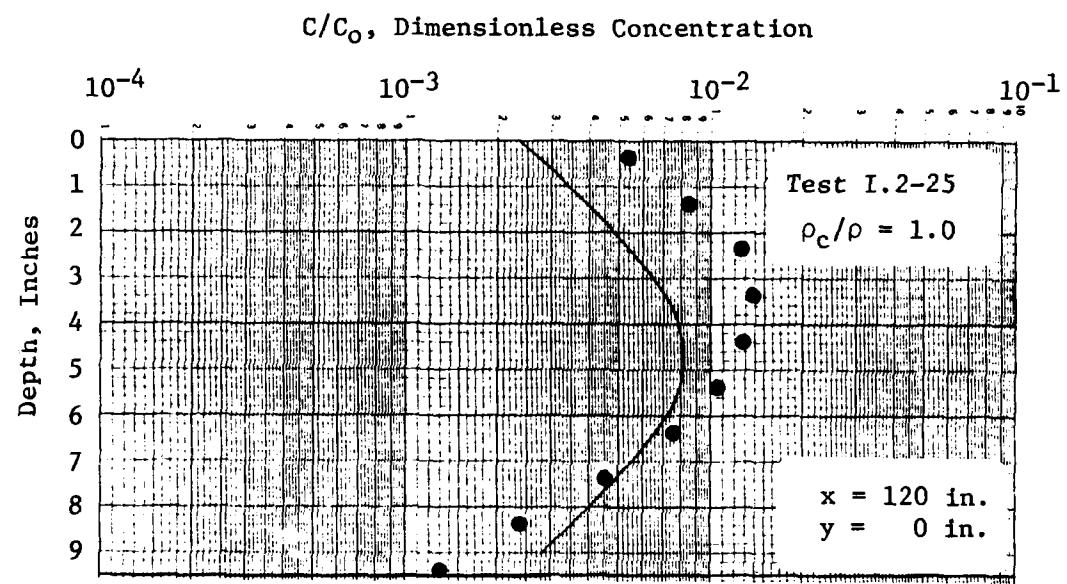
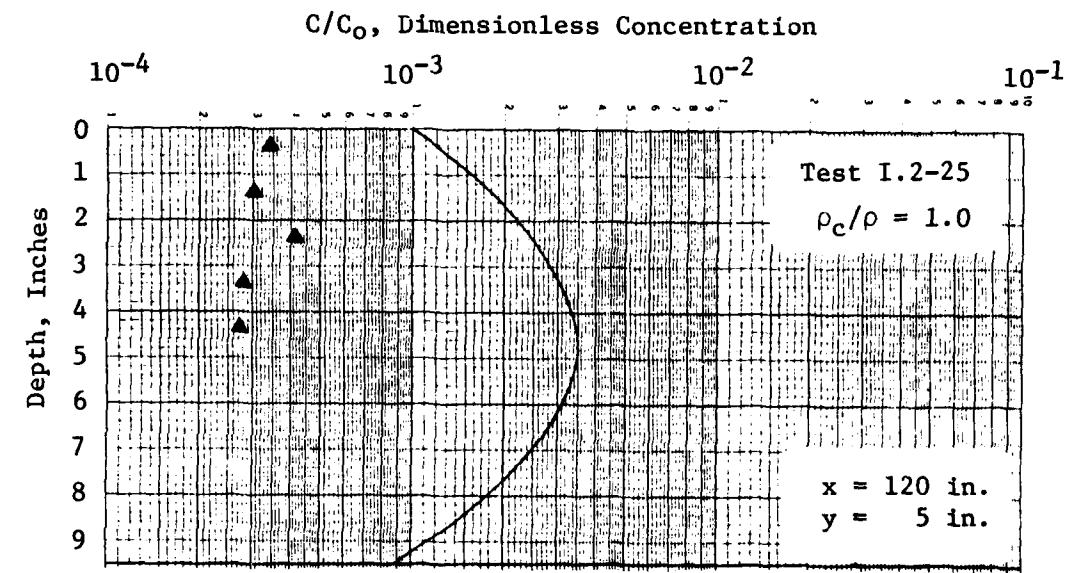


FIGURE V.4 VERTICAL CONCENTRATION PROFILES FOR CONTINUOUS SPILL
OF NEUTRALLY BUOYANT CHEMICAL

conclude from this comparison that the plume models predict fairly well the correct concentration distribution for neutrally buoyant discharges. Agreement can be improved further by optimizing the values of α_1 and α_3 for best fit.

Figures V.5 to V.9 compare model predictions and data for Run L.2-12, a continuous discharge of sucrose and dye with s.g. = 1.05. Figure V.5 shows very good agreement between the predicted plume boundary ($y = B_{eff}$) and the observations of flow visualization. Figure V.6 compares the plume centerline concentration predictions at $y = 0$ and $z = d$ with data. The agreement is good for $x > 5$ meters. At lower distances the plume was slightly bifurcated and the centerline concentration was lower than on the side lobes. Figure V.7 shows that the predicted values of S_z agree fairly well with experimental values of S_z obtained from the concentration profile data. Figures V.8 and V.9 show predicted and measured cross-stream concentration profiles at 1.21m (48 inches) and 3.05m (120 inches). The overall agreement is good, although the plume model does not simulate the bifurcated profile exactly.

Figures V.10 to V.14 compare model predictions and data for Run I.2-20, a continuous discharge of sodium silicate and dye with s.g. = 1.40. Since the Froude number associated with this release is < 0.6 , the chemical pool spreading model is used. As described in Section III.2.3, this model assumes that the plume of diluted chemical forms a pool over the bottom of the channel. The equilibrium size of the pool is determined by a balance between the mass flow rate into the pool, given by Equation III.33, and the rate of entrainment (or uptake) of chemical solution into the flowing water stream above the pool, given by Equation III.34. As shown in Figure III.3, the pool is assumed to be square in shape with dimensions of $L \times L, m^2$. Gravity spreading of the entrained chemical is assumed to begin at the downstream pool boundary at $x = L/2, m$.

Figure V.10 compares the predicted plume boundary above the floor of the channel with data obtained from observations of the plume boundary during flow visualization. As shown in this figure, the plume model predicts a square area source with $L \sim 1.28m$. Downstream of the source area, the

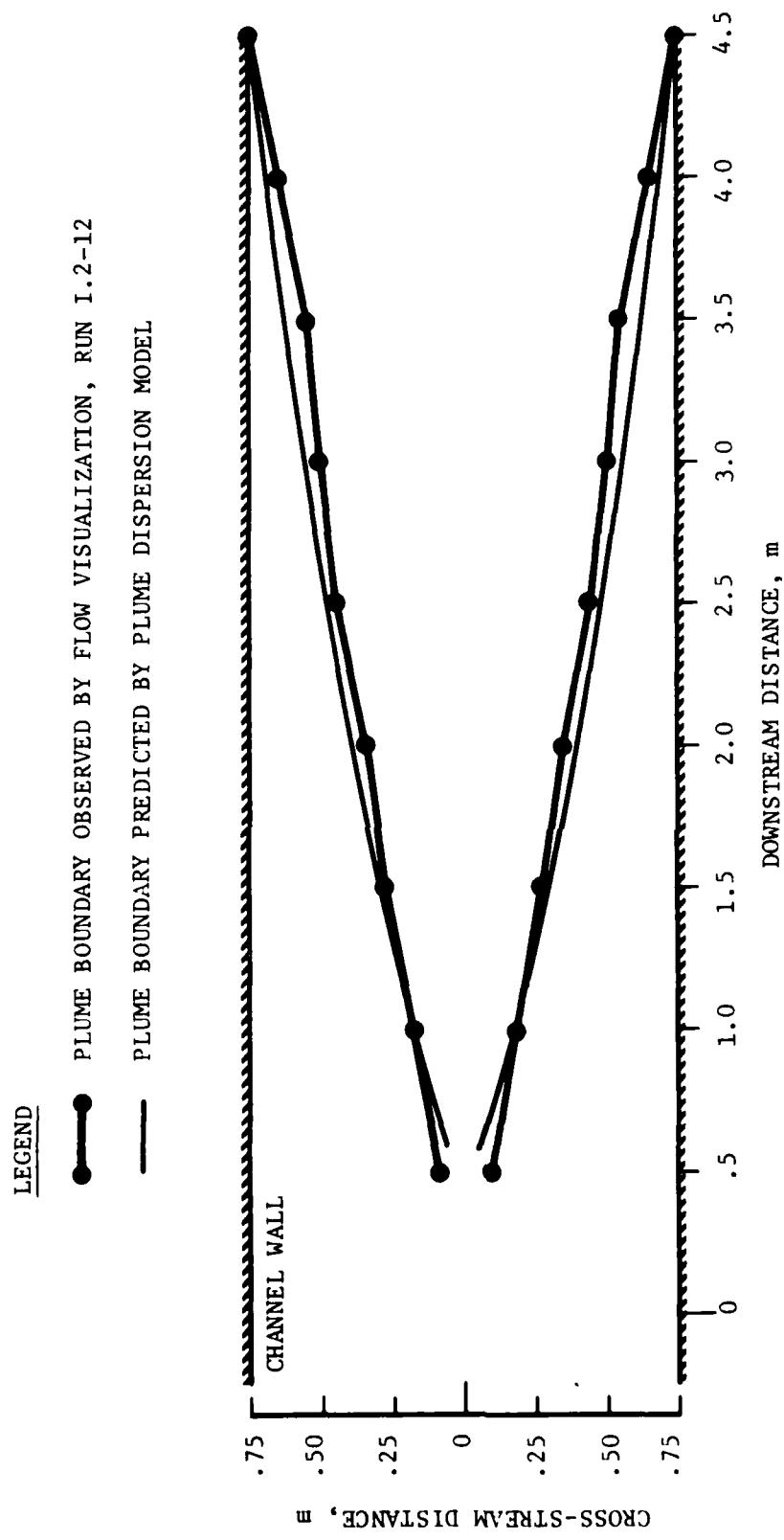


FIGURE V.5 PLUME BOUNDARY FOR SUCROSE, $s.g. = 1.05$ AT $z = 0.24\text{m}$
(CHANNEL BOTTOM)

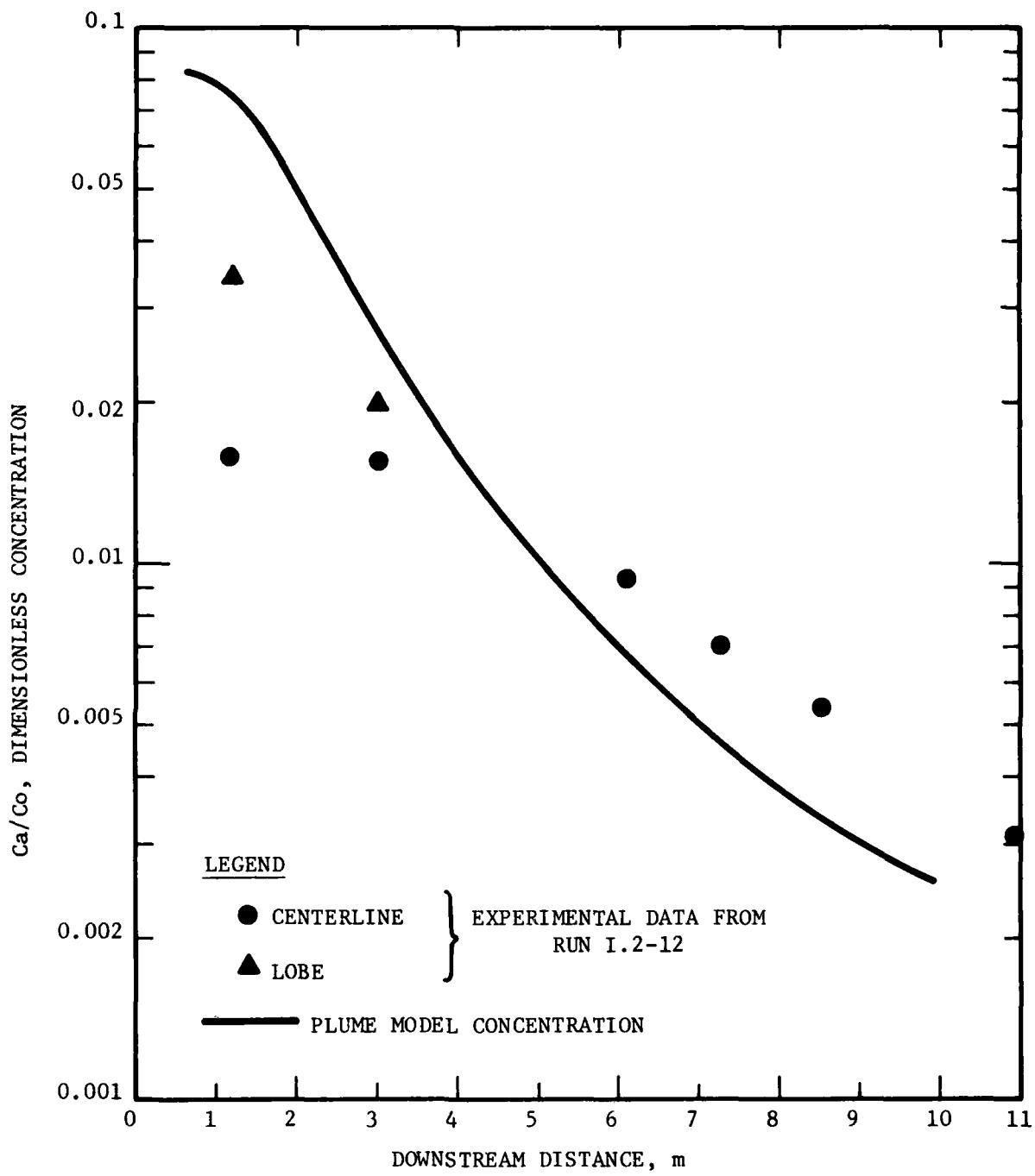


FIGURE V.6 PREDICTED AND MEASURED VALUES OF PLUME CENTERLINE CONCENTRATION FOR SUCROSE, s.g. = 1.05

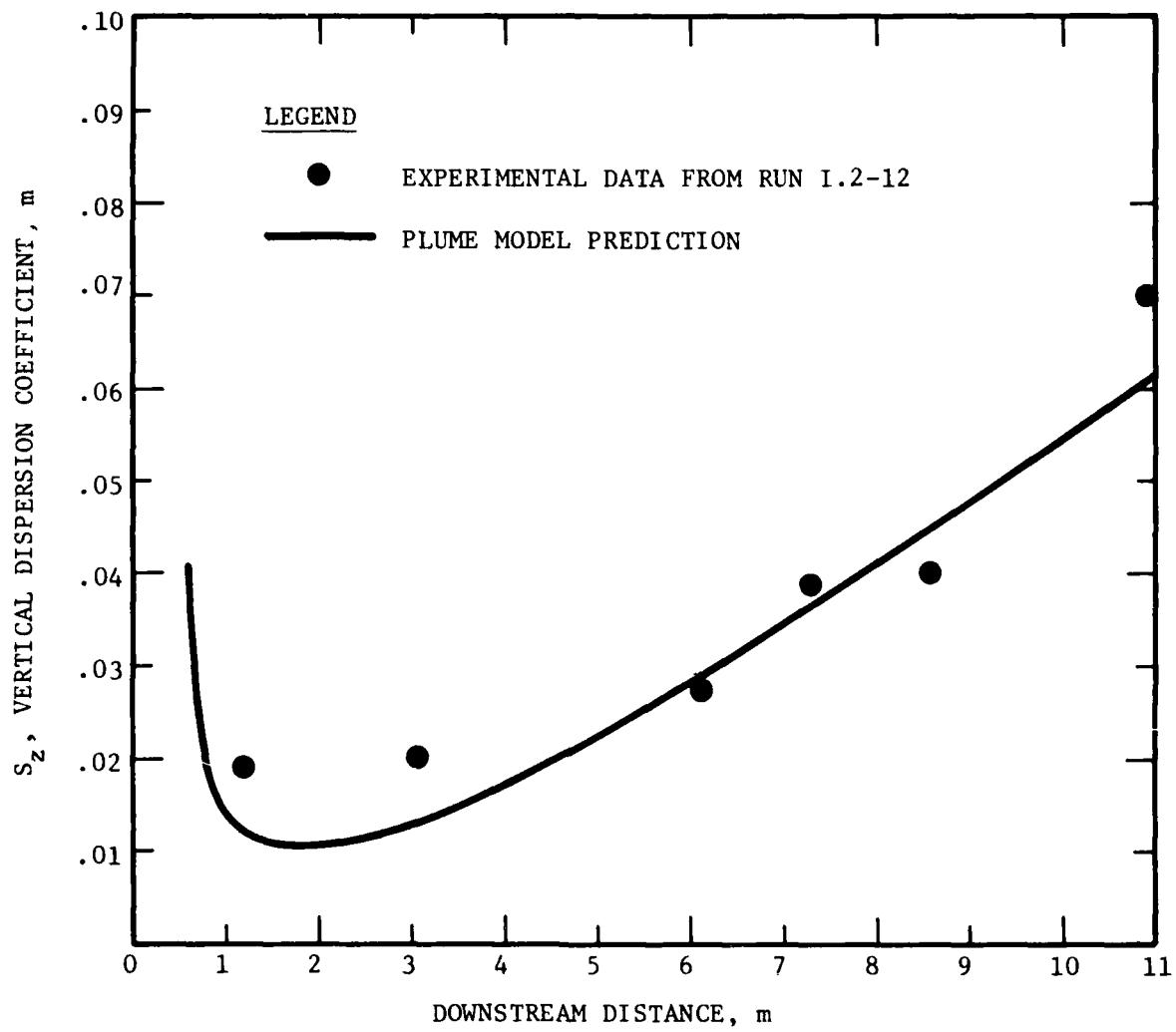


FIGURE V.7 PREDICTED AND MEASURED VALUES
OF S_z FOR SUCROSE, s.g. = 1.05

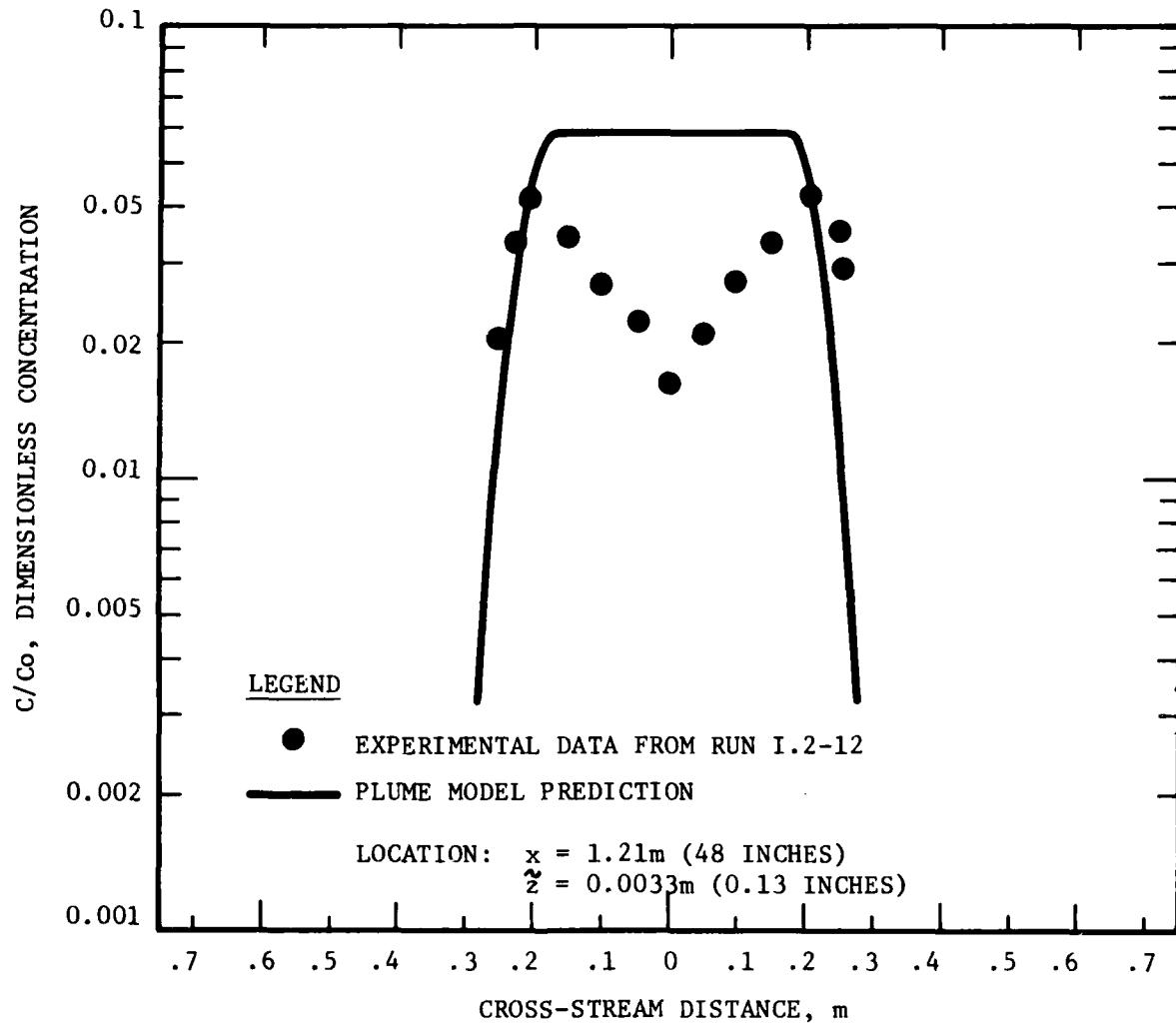


FIGURE V.8 CROSS-STREAM CONCENTRATION PROFILE AT
 $x = 1.21\text{m}$ (48 INCHES) FOR SUCROSE, s.g. = 1.05

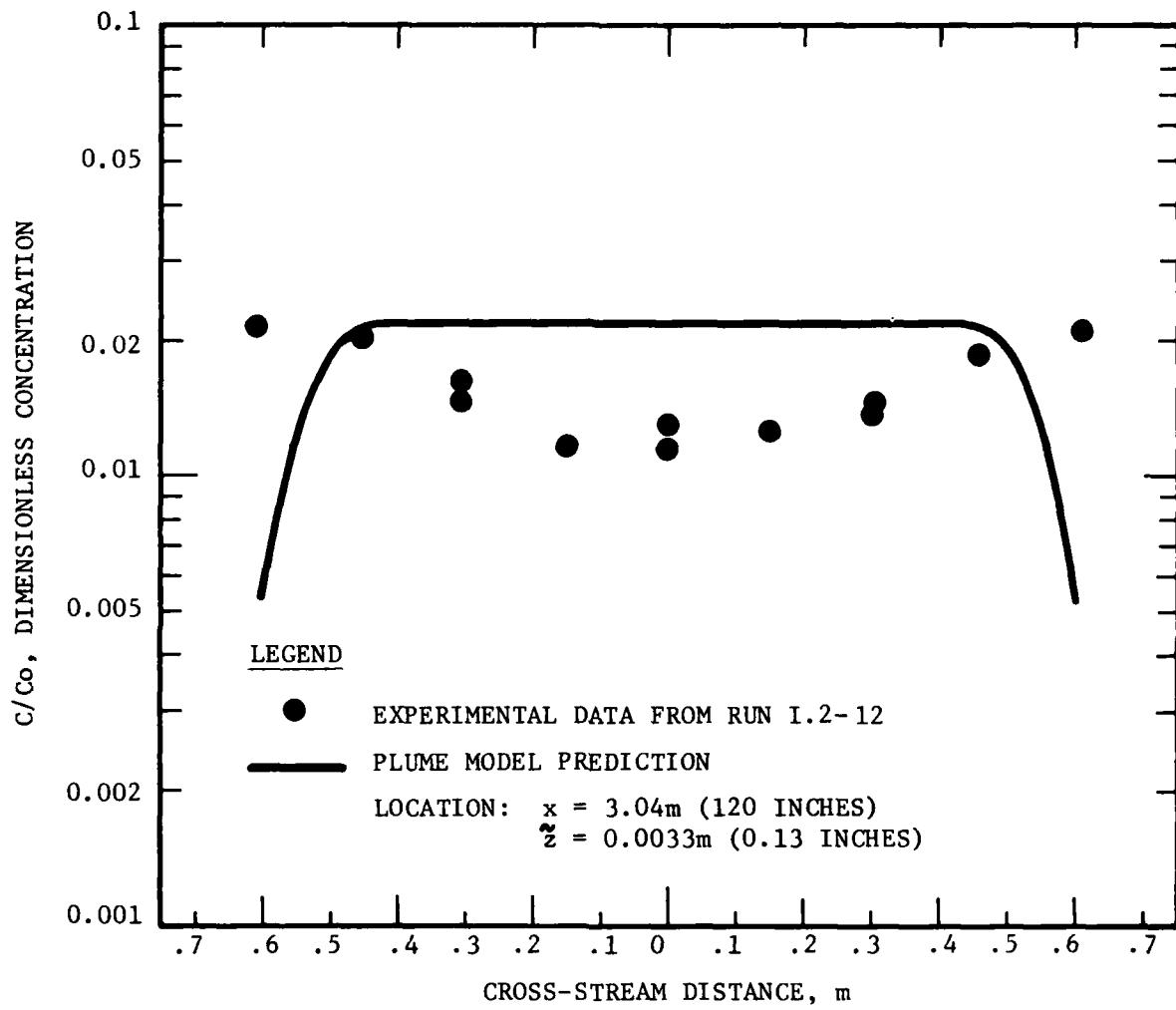


FIGURE V.9 CROSS-STREAM CONCENTRATION PROFILE AT
 $x = 3.04\text{m}$ (120 INCHES) FOR SUCROSE, s.g. = 1.05

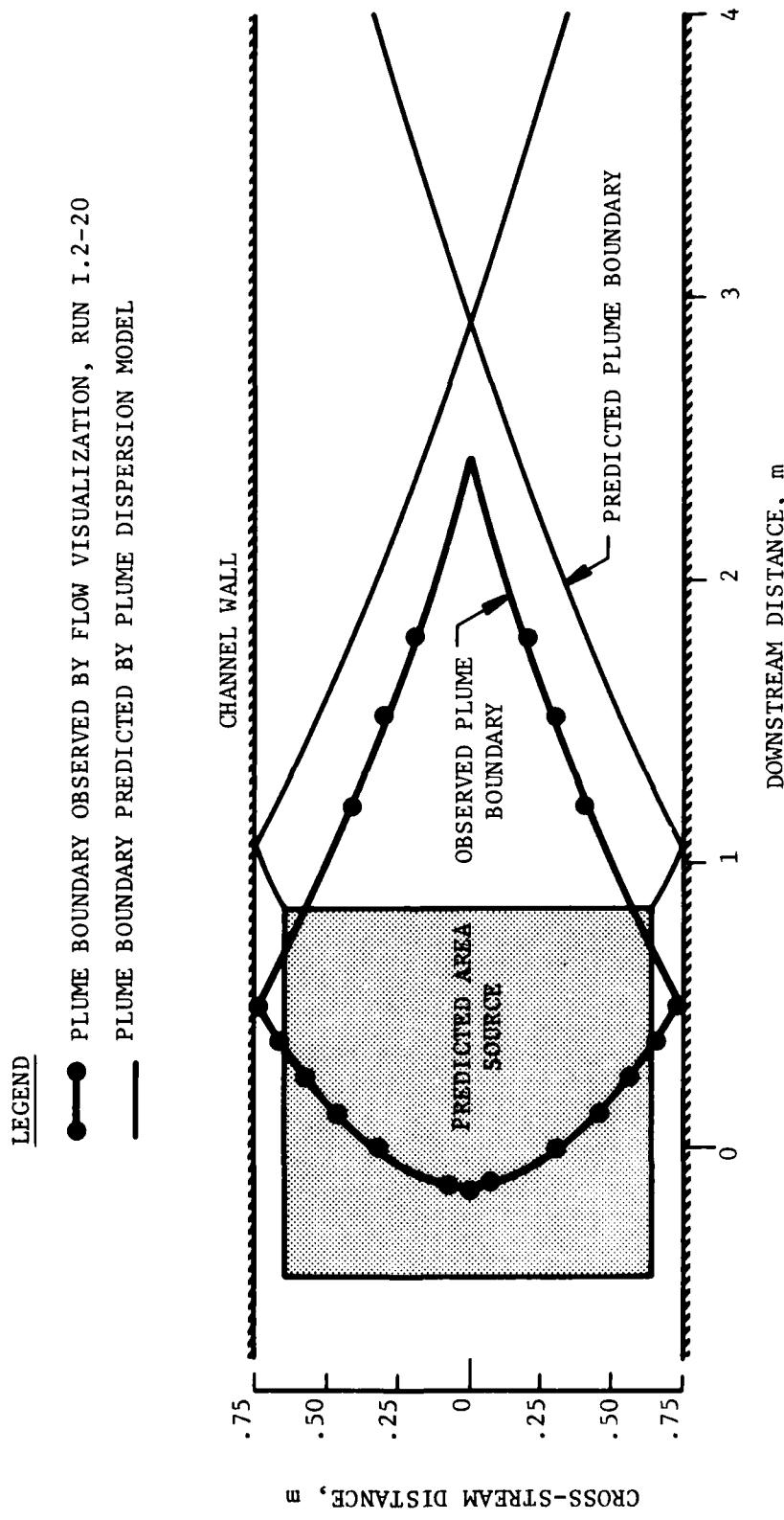


FIGURE V.10 PLUME BOUNDARY FOR SODIUM SILICATE, s.g. = 1.40 AT $z = 0.24\text{m}$
(CHANNEL BOTTOM)

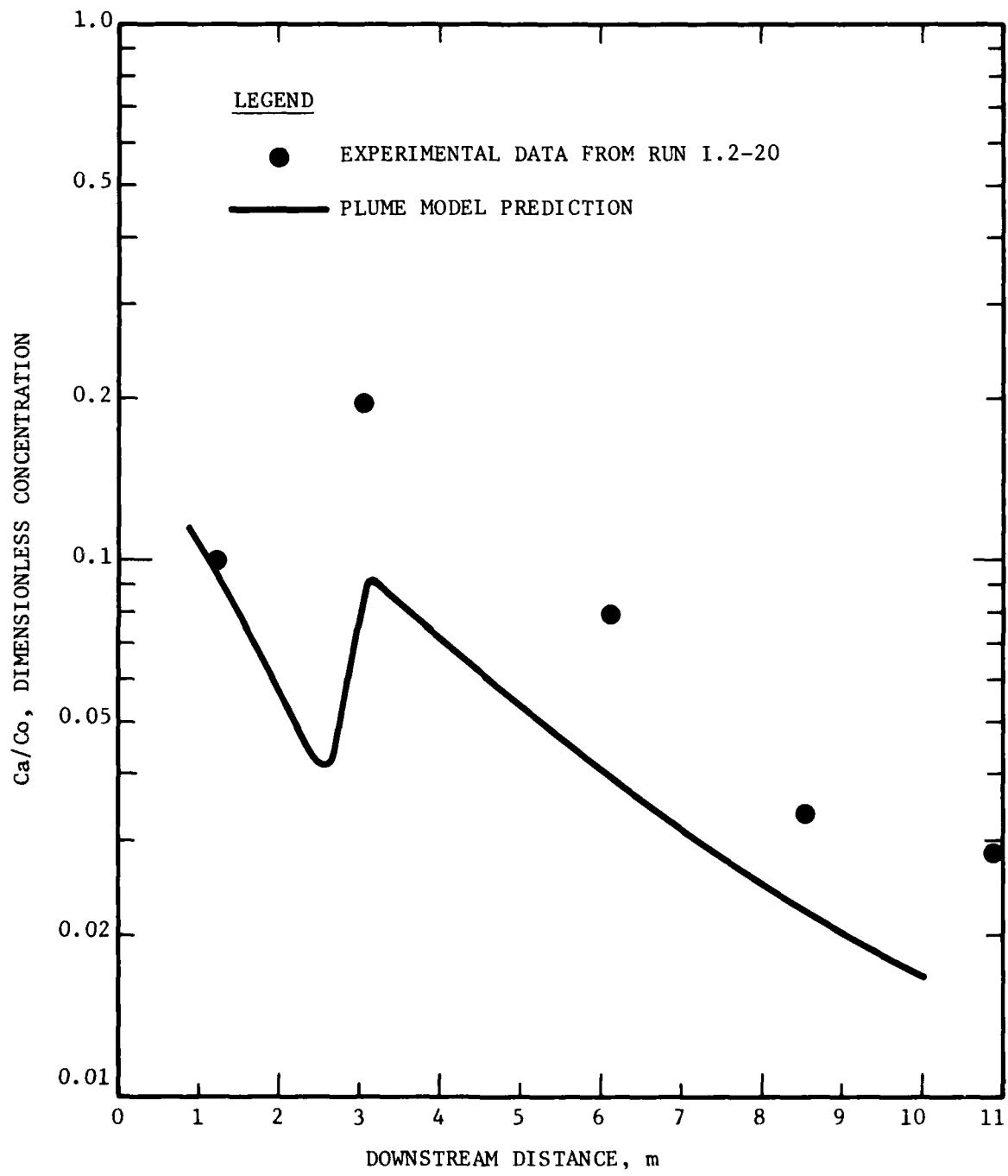


FIGURE V.11 PREDICTED AND MEASURED VALUES OF PLUME CENTERLINE CONCENTRATION FOR SODIUM SILICATE, s.g. = 1.40

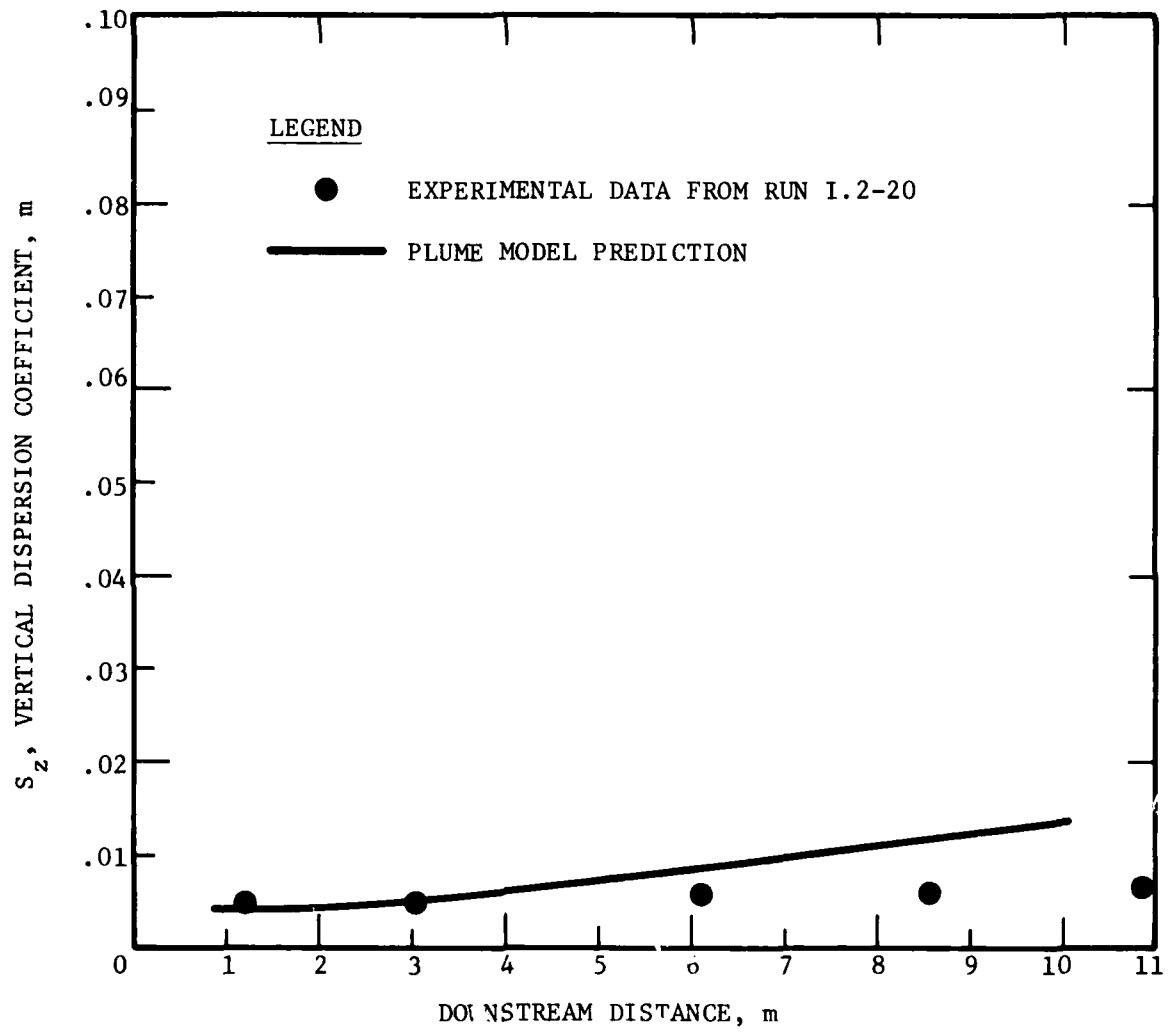


FIGURE V.12 PREDICTED AND MEASURED VALUES
OF S_z FOR SODIUM SILICATE, s.g. = 1.40

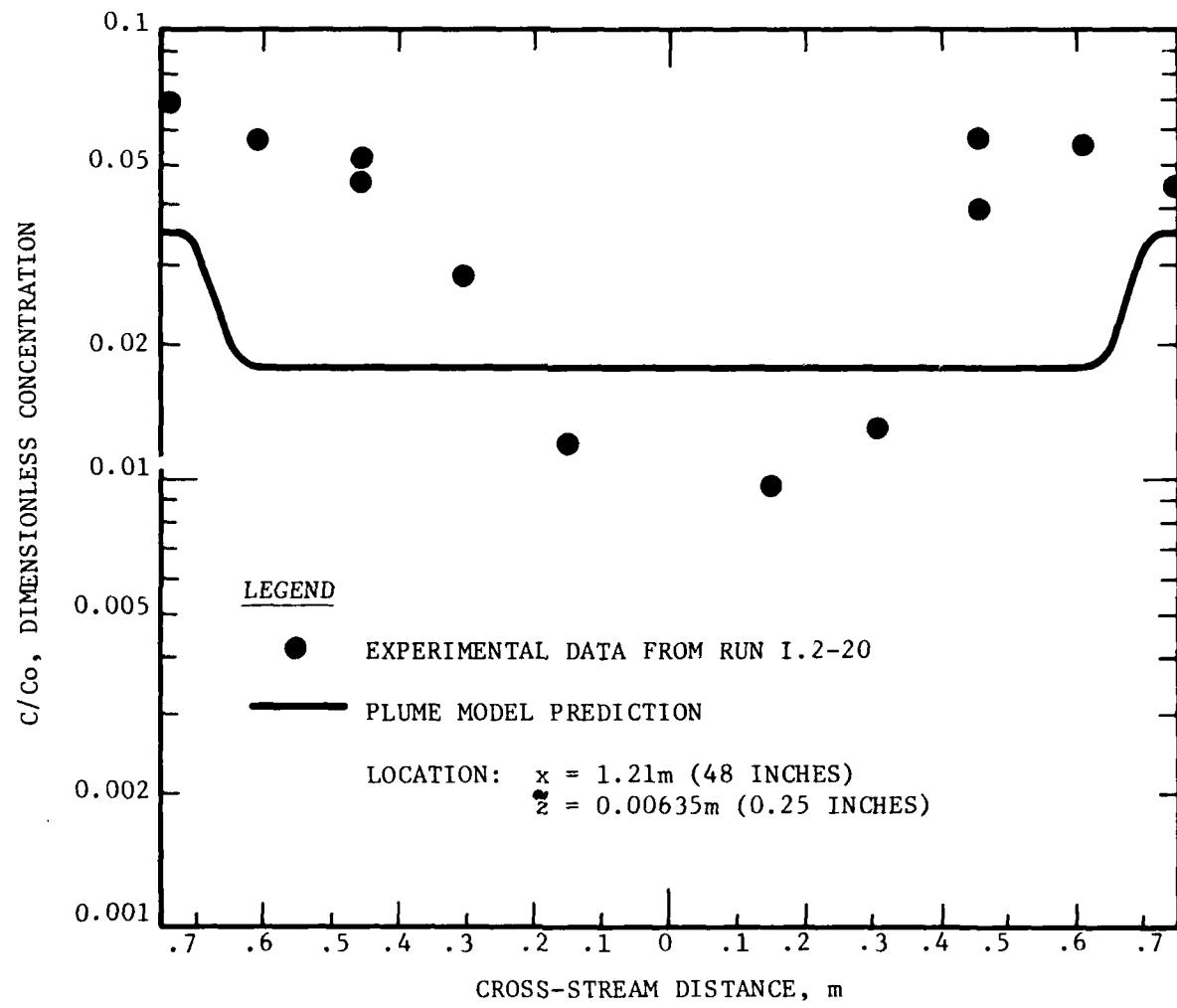


FIGURE V.13 CROSS-STREAM CONCENTRATION PROFILE AT
 $x = 1.21\text{m}$ (48 INCHES) FOR SODIUM SILICATE, s.g. = 1.40

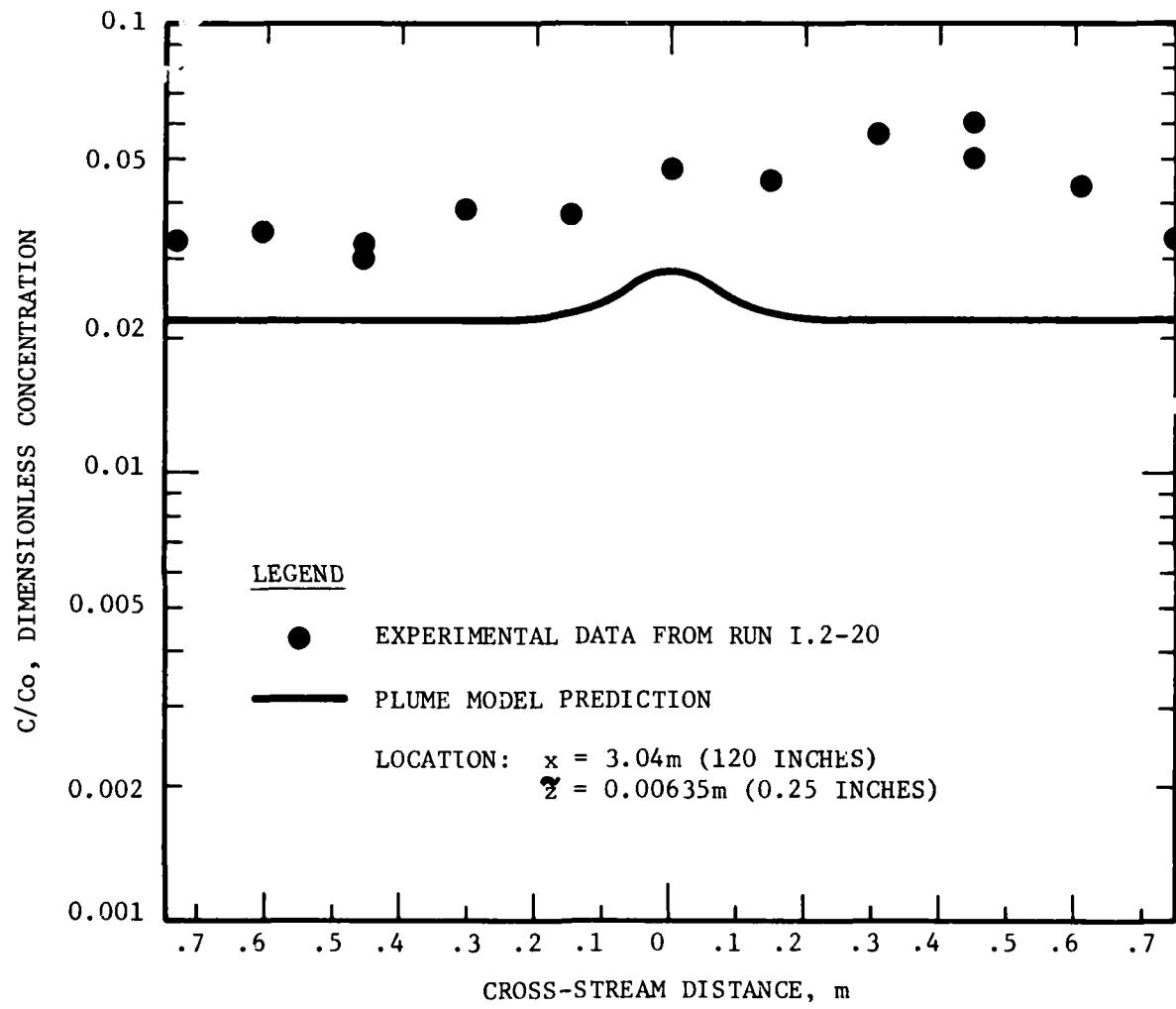


FIGURE V.14 CROSS-STREAM CONCENTRATION PROFILE AT
 $x = 3.04\text{m}$ (120 INCHES) FOR SODIUM SILICATE, s.g. = 1.40

plume boundary ($y = B_{eff}$) is predicted to reach the channel walls at $x = 1.05m$. At this location the plume boundary reflects back towards the plume center. The model predicts that the reflections cross in the center of the channel at $x = 2.93m$.

Flow visualization tests revealed a somewhat different behavior as shown in Figure V.10. The area source did not extend as far upstream as predicted by the model, and lateral gravity spreading of entrained chemical occurred above the pool. As a result, the plume boundary reached the channel wall at $x = 0.5m$ instead of at $1.05m$ as predicted by the model. Flow visualization photographs did show a reflection of the plume boundary at the channel walls. The reflections merged at approximately $x = 2.45m$ instead of at $2.93m$ as predicted by the model. However, the plume dispersion model with chemical pool formation at low values of Froude number gives a representation of actual plume behavior that is approximately correct.

Figures V.11 and V.12 show that the plume centerline concentration and the vertical dispersion coefficient (a measure of plume thickness) are fairly well predicted by the plume model. The vertical concentration profile data obtained along the channel centerline for Run I.2-20 indicate that the plume is thinner and less dilute than predicted by the plume model. Figures V.13 and V.14 compare the predicted and measured cross-stream concentration distributions at a height of $0.0064m$ (1/4 inch) above the channel floor at downstream distances of $x = 1.21m$ and $x = 3.04m$, respectively. The effect of plume boundary reflection from the channel wall is easily seen in Figure V.13. In general, the agreement is good, although the plume model has predicted a greater dilution (by a factor of 2) for the sodium silicate experiment.

Figures V.15 to V.19 compare model predictions and data for Run 1.2.4, a continuous discharge of ethanol and dye with $s.g. = 0.79$; the plume for this test runs along the water surface rather than the channel bottom. This plume was bifurcated near the source. Figure V.15 shows that the predicted plume boundary lies between the inner and outer boundaries of each lobe of the bifurcated plume. Because of the bifurcation, the predicted centerline concentration is much greater than the observed one, as is shown in Figures V.16, V.18, and V.19, although the predicted trend is accurate. The vertical

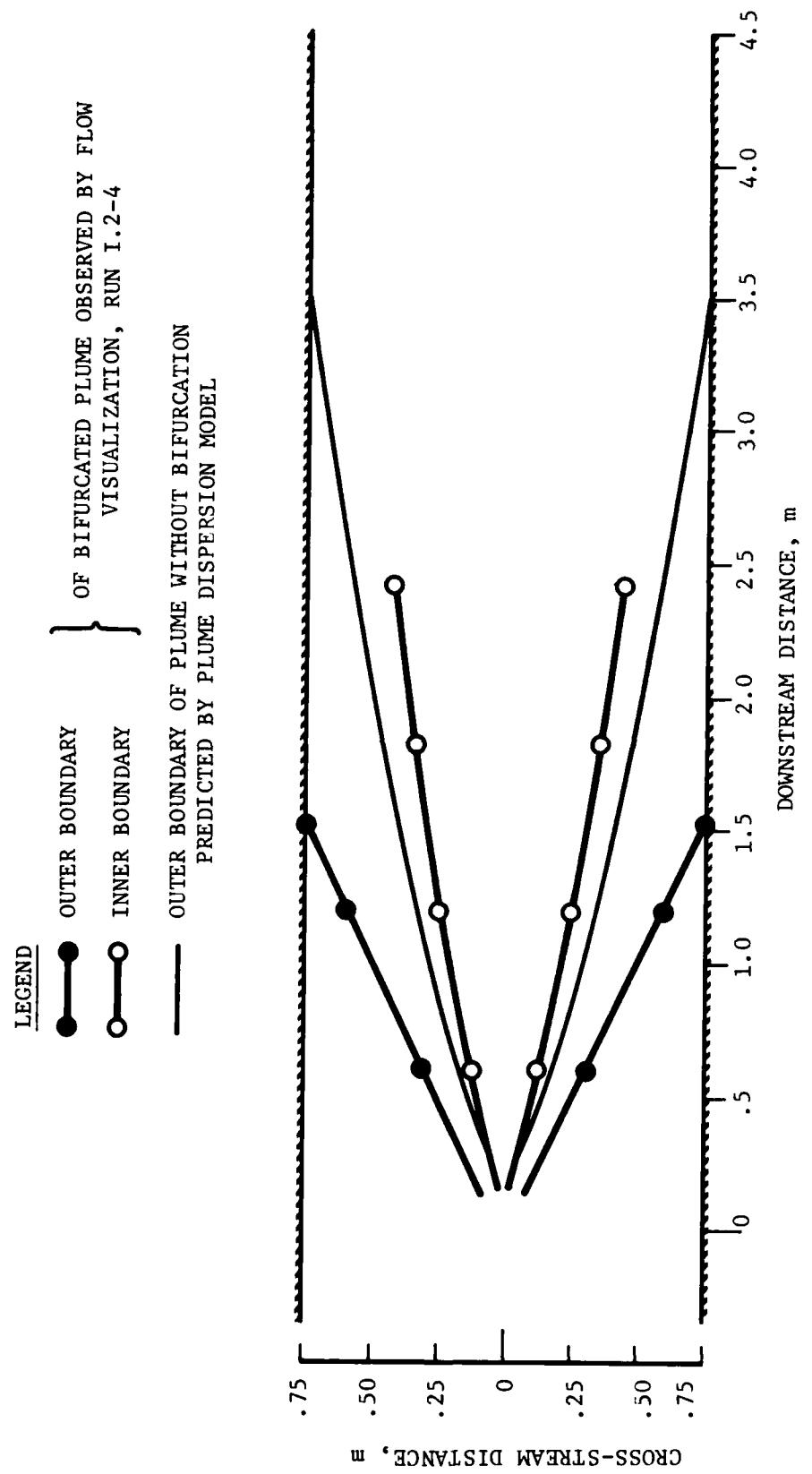


FIGURE V.15 PLUME BOUNDARY FOR ETHANOL, s.g. = 0.79
at $z = 0$ m (CHANNEL SURFACE)

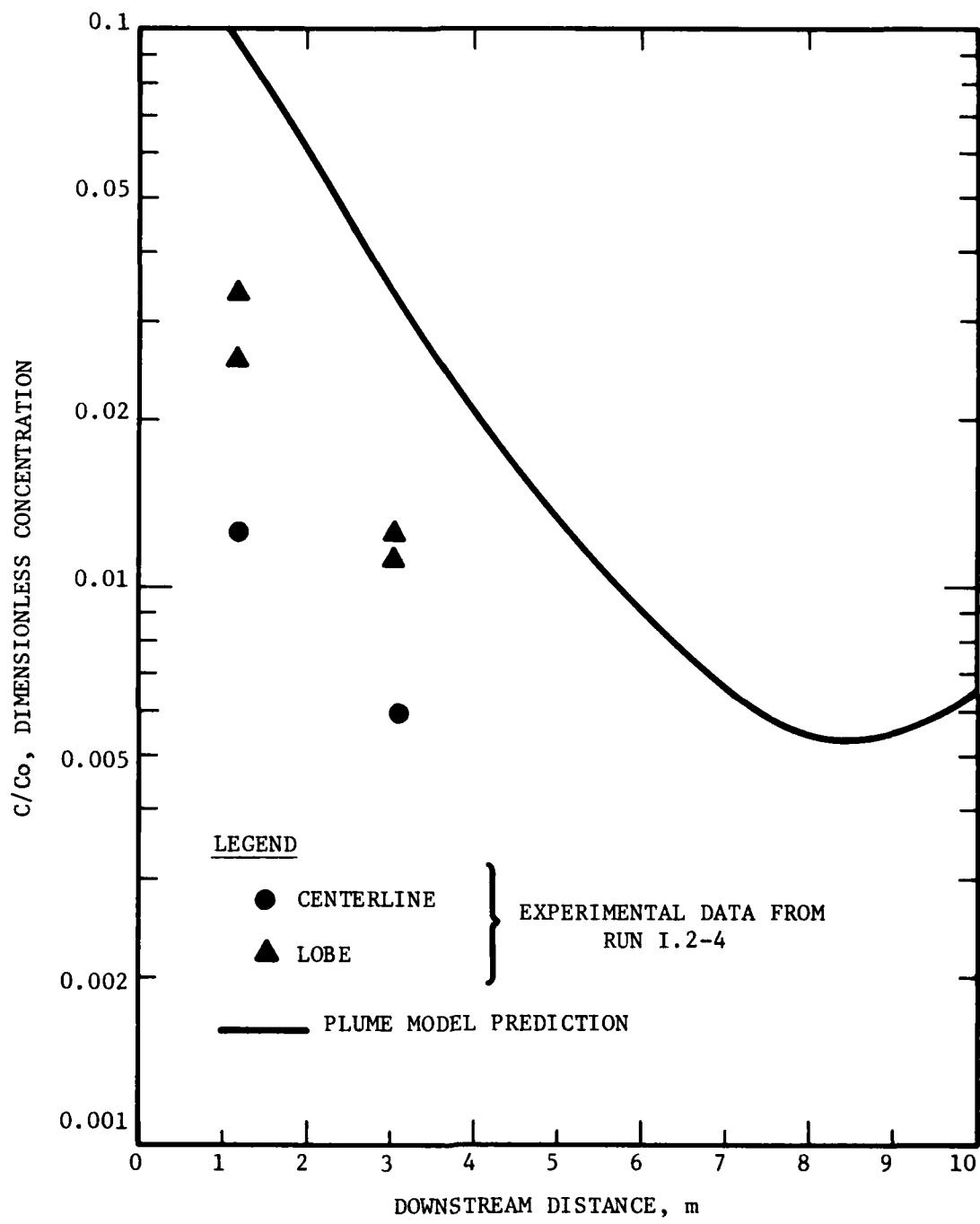


FIGURE V.16 PREDICTED AND MEASURED VALUES OF PLUME CENTERLINE CONCENTRATION FOR ETHANOL, s.g. = 0.790

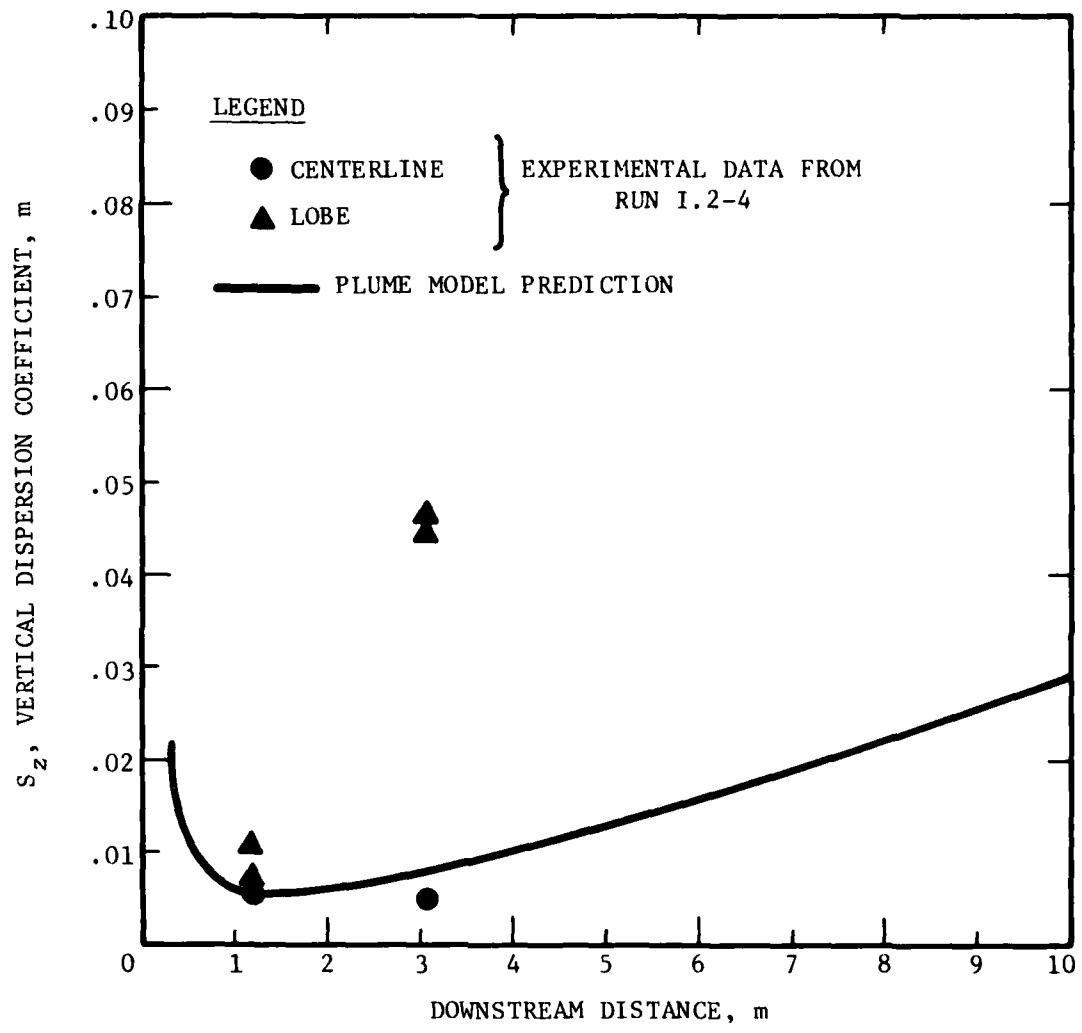


FIGURE V.17 PREDICTED AND MEASURED VALUES
OF S_z FOR ETHANOL, s.g. = 0.79

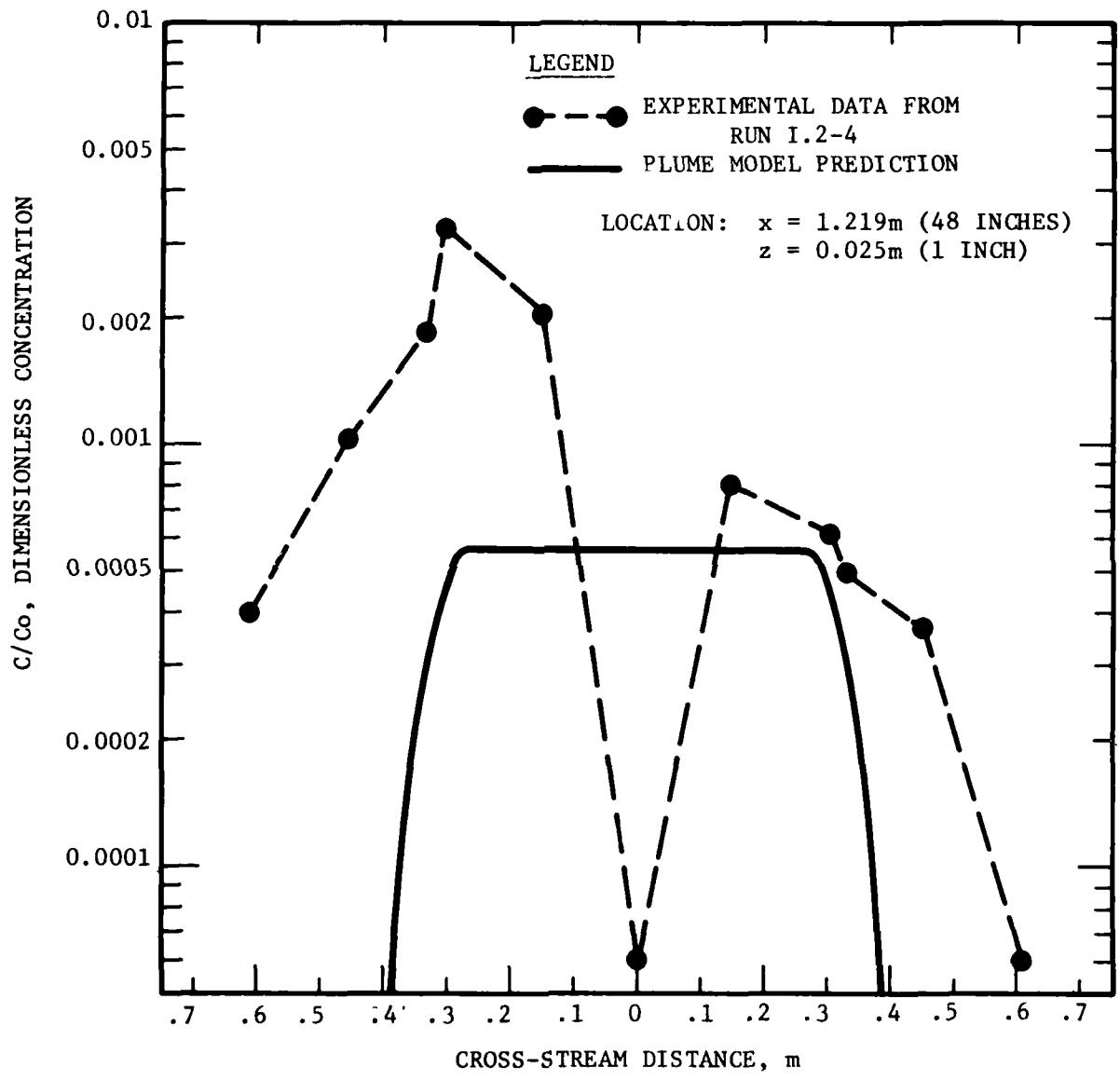


FIGURE V.18 CROSS-STREAM CONCENTRATION PROFILE FOR ETHANOL,
s.g. = 0.79 at $x = 1.219\text{m}$ (48 INCHES),
 $z = 0.025\text{m}$ (1 INCH)

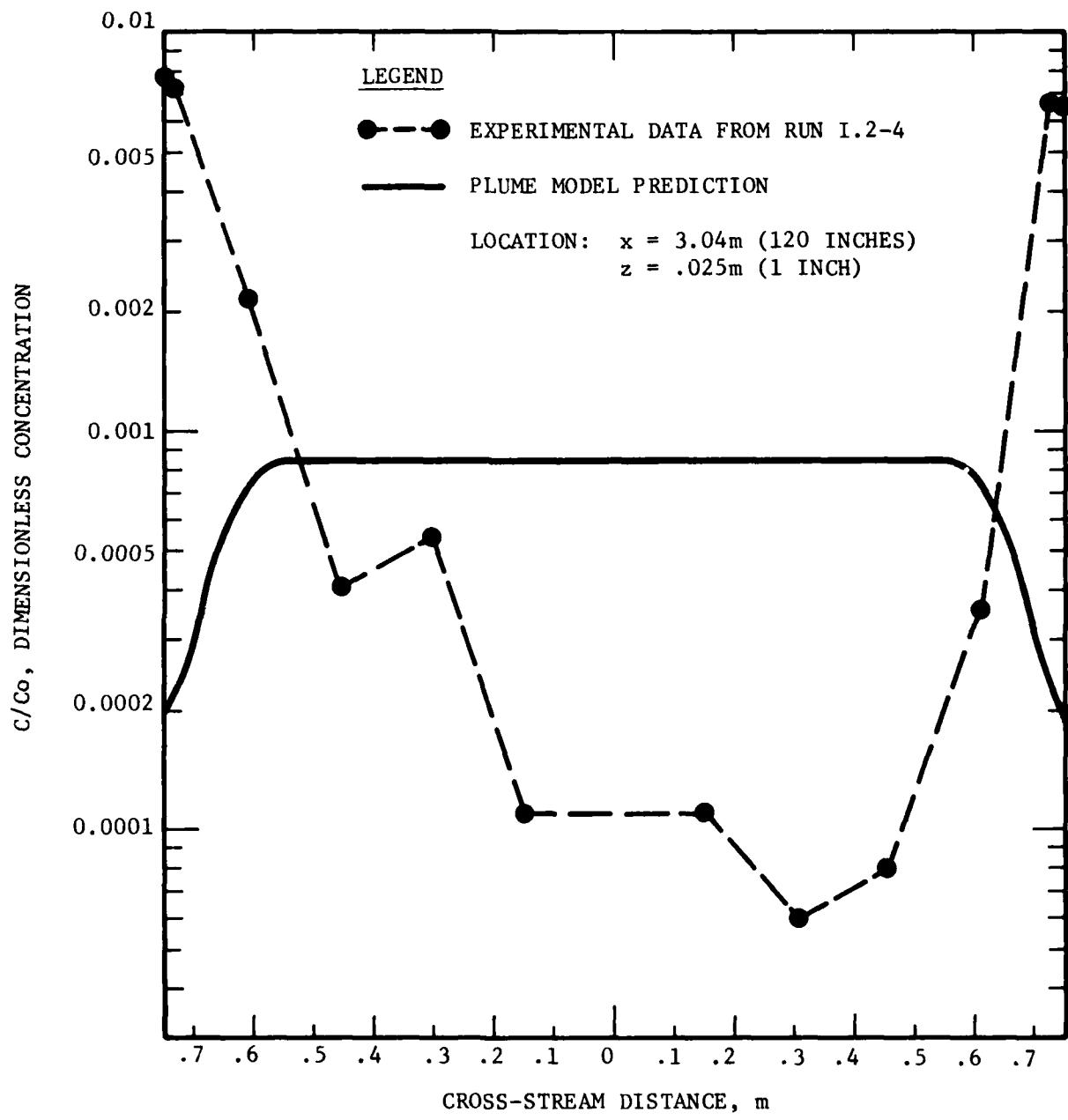


FIGURE V.19 CROSS-STREAM CONCENTRATION PROFILE AT
 $x = 3.04\text{m}$ (120 INCHES) FOR ETHANOL, s.g. = 0.79

concentration distribution data taken within the two lobes of the plume at $x = 1.21m$ and $x = 3.04m$ gave noticeably higher values of concentration at the water surface. However, these values are still well below the values predicted for the plume centerline.

Figure V.17 compares predicted and measured values of the vertical dispersion coefficient, a measure of plume thickness. The agreement was reasonably good at $x = 1.21m$, but at $x = 3.04m$ the thickness of the lobes (determined from vertical concentration profiles taken next to the channel walls) is much greater than the predicted thickness. Figures V.18 and V.19 compare the predicted and measured cross-stream concentration distributions at a depth of $0.025m$ (1 inch) below the water surface. The effect of the bifurcation is clearly shown in these figures. The high values of concentration within the plume lobes at this depth are the result of the greater values of plume thickness indicated in Figure V.17. While the measured values of concentration at the surface ($z = 0$) are lower than predicted (see Figure V.16), the values at $z = 0.025m$ below the surface are higher than predicted. The prediction of the chemical concentration distribution for this case involving strong plume bifurcation is perhaps the least satisfactory of all the continuous spill tests.

V.2 Instantaneous Spills in Steady Rivers

Predictions of the model are first compared to the tests of a neutrally buoyant spill, Case II.1-20. (Mass spilled = 0.9 kg ; spill location $z = d/2 = 0.114m$; channel velocity = $0.141m/\text{sec.}$) Figure V.20 shows a comparison of the observed and predicted peak concentrations of the spill as a function of time, at a downstream location of $5.36m$. The model agrees well with the data. These predictions correspond to the near-field, point-source regime in which turbulent diffusion is the dilution mechanism. Initially, the model was based on a longitudinal diffusion coefficient, ϵ_x , that was equal to the lateral coefficient ϵ_y ; this gave a time duration of the spill that was too short at the measurement location by a considerable margin (i.e., the curve was too "peaked"). By iteration, it was found that $\epsilon_x = 10 \epsilon_y$ gave much better agreement.

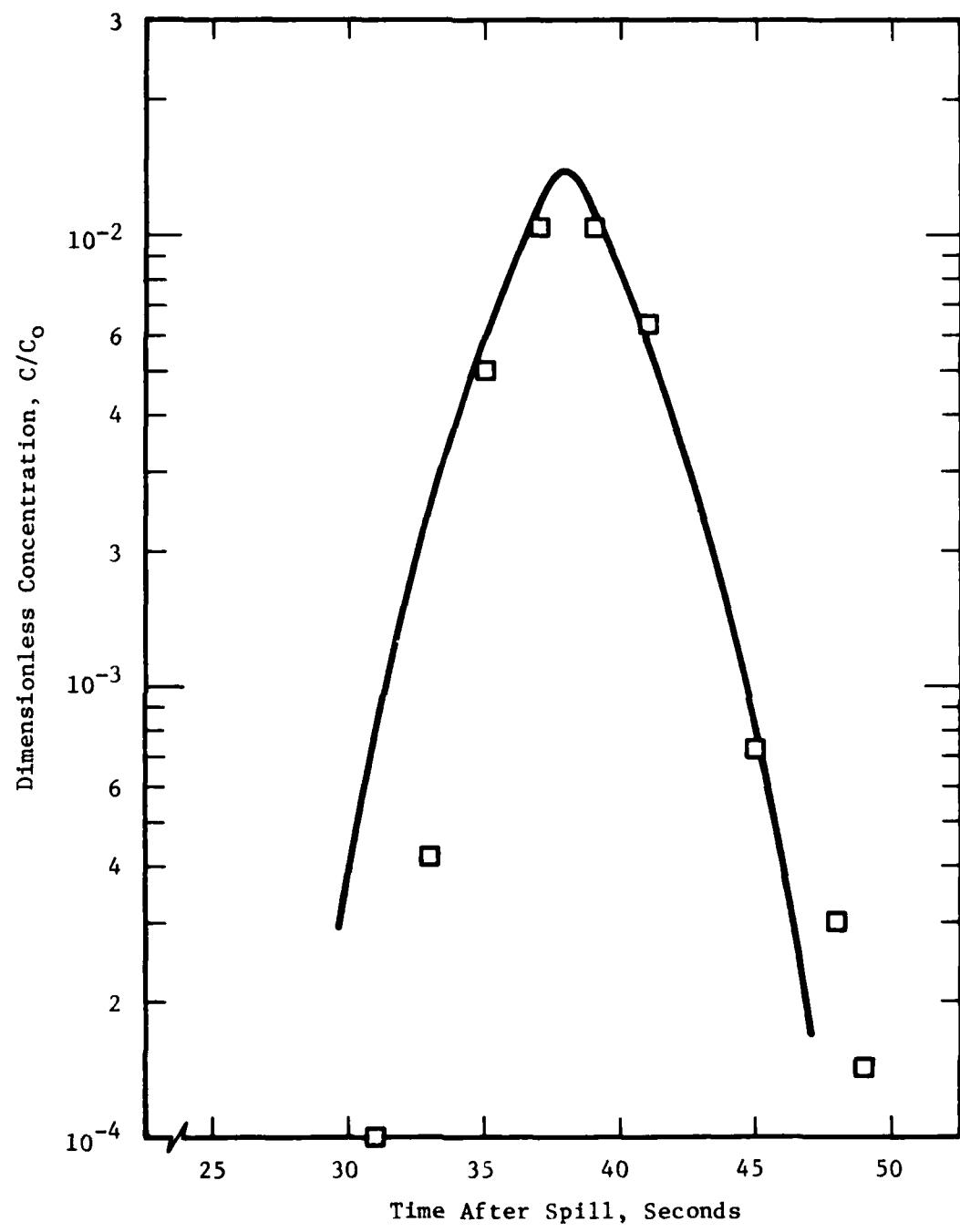


FIGURE V.20 CONCENTRATION VS. TIME AT
 $x = 5.36\text{m}$ (211 in.) AND
 $z = 0.032\text{m}$ (1.25 in.) FOR
WATER + DYE, s.g. = 1.0

The predicted concentration across the channel depth also compares well with the data, as shown in Figure V.21. When $\epsilon_x = \epsilon_y$ was used initially, however, the predicted distribution was nearly constant over the depth, which is a consequence of the conservation of spilled mass. That is, if the spill is too short in the longitudinal direction, as it would be when $\epsilon_x = \epsilon_y$, the concentration must average out as too high over the depth in order to make up the mass discrepancy. Further, Figure IV.27 of Section IV demonstrated photographically that the spill diffuses more rapidly in the longitudinal direction than in the lateral direction. (The use of $\epsilon_x = 10 \epsilon_y$ rather than $\epsilon_x = \epsilon_y$ also results in more realistic concentration profiles for the positive- and negative-buoyancy spills that will be discussed later. According to Fischer [5], values of ϵ_x greater than ϵ_y are to be expected.) Note that, although Case II.1-20 is nominally a neutrally-buoyant spill, a slight temperature difference between the spilled water-plus-dye and the channel water resulted in the spill's rising to the surface; this fact has been used in the model predictions.

Figures V.20 and V.21 have been prepared on the basis of a time comparison rather than on downstream distance. In the model, the predicted downstream distance corresponding to the peak concentration is 5.36m (211 in.), which is the product of the channel current and the time. The actual measurements were taken, however, at 4.27m (168 in.). Since the model and the data compare fairly well for the test observation time of 38 seconds (the peak concentration time) it is concluded that the difference in downstream distance is a result of the difficulties in (1) obtaining an ideal "instantaneous" discharge as well as in (2) measuring the current exactly. This same kind of discrepancy between time and distance appears in all the comparisons given below. For that reason, the comparisons will always be made on the basis of the time elapsed from when the spill was injected into the channel.

Comparisons are next made to a spill of sodium silicate with a specific gravity of 1.40. (Case II.1.14; mass spilled = 1.29 kg; spill location $z = d/2 = 0.114$ m; channel velocity = 0.141 m/sec). Because the spill was strongly negatively-buoyant, it had an extended region of buoyancy-induced

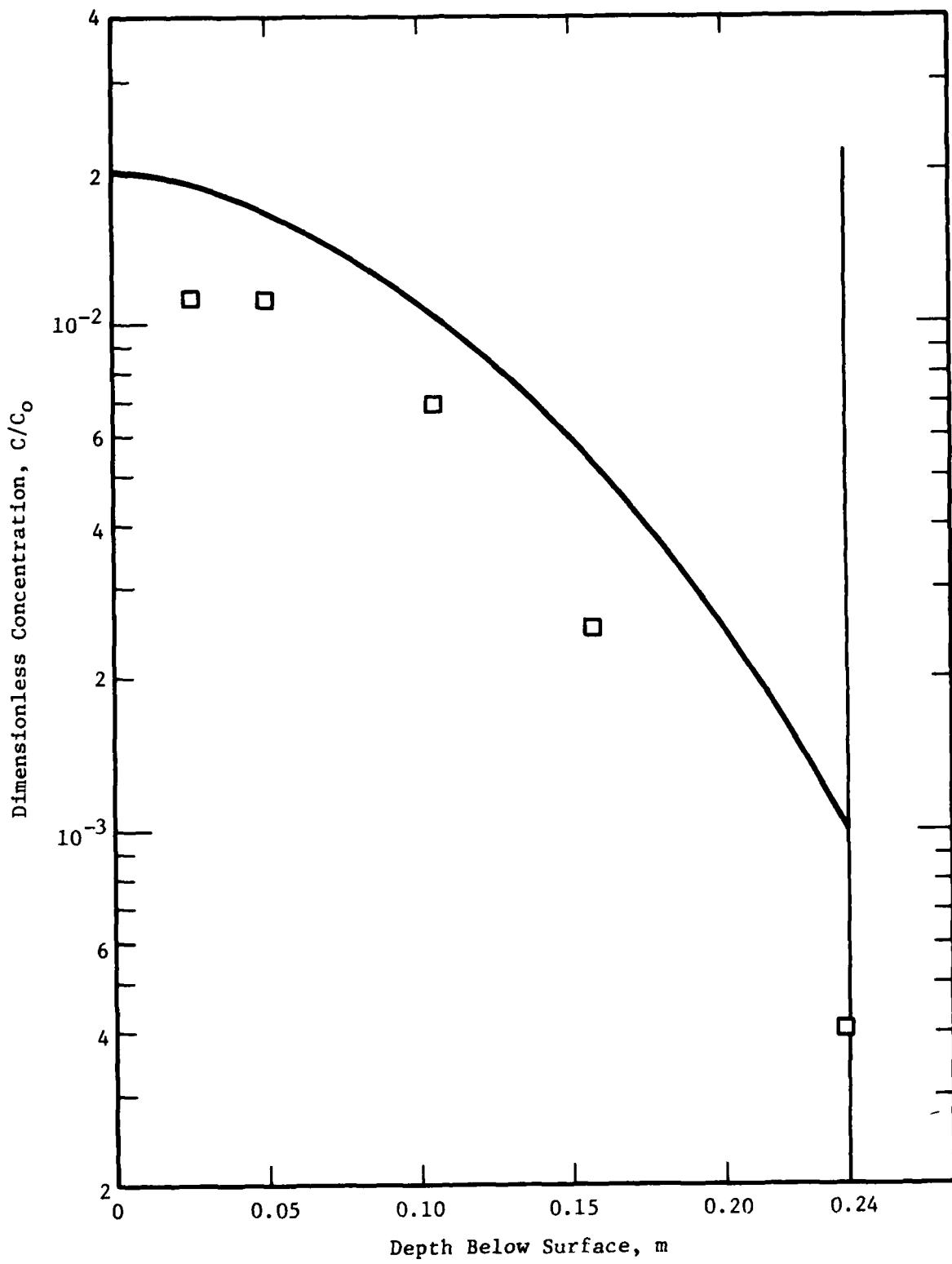


FIGURE V.21 CONCENTRATION VS. DEPTH AT
 $x = 5.36\text{m}$ (211 in.) AND
 $t = 32$ seconds FOR
WATER + DYE, s.g. = 1.0

mixing. Figure V.22 shows a comparison of the measured and predicted concentrations at the channel centerline as a function of time for a downstream location of 5.02m. (As discussed above, $x = 5.03m$ corresponds to a test time of 36 seconds, when the center of the actual cloud was observed, not to the actual measurement location of 4.27m.) The spill bifurcated noticeably after it impacted the channel floor, as can be seen in the photographs of Figure IV.26. For that reason, the measured peak concentrations (off the centerline) are also shown in Figure V.22. The predictions, which do not include any effects of bifurcation, generally lie between the centerline and the peak data. Since the model predicts that the spill is in the very-near-field regime, the predicted concentration increases abruptly to a maximum when the leading edge of the "top hat" profile reaches the measurement location. After that, the predicted concentration gradually decreases as a result of further dilution during the time required for the cloud to pass by the measurement location. The actual spill diffuses somewhat both upstream and downstream, so the measured concentration does not change discontinuously. Nonetheless, the agreement between model and test is satisfactory.

Figure V.23 compares the predictions of the concentration across the channel width at $t = 26$ seconds to the measured data. The bifurcation of the actual spill is evident. The model predicts that (1) the cloud extends completely across the channel, in agreement with the data, and (2) the concentration is uniform; altogether the comparison is reasonably good.

Comparisons of the predicted concentration through the water depth at $t = 26$ seconds are shown in Figure V.24. The measured concentration decreases from a peak to practically zero over the lower 0.05m of the channel, thus verifying that the cloud is still stratified and mixing by buoyancy, as the model predicts. For the model, the top-hat profile decreases to zero over the bottom 0.015m; since this range includes nearly all the mass of the actual spill, the agreement is considered satisfactory. Also shown in Figure V.24 are comparisons (the dashed lines) of the predictions of the very-near-field and the near-field models near their matching points, $t \approx 49$ seconds. The near-field model gives a ten-to-one concentration decrease over the channel depth, while the very-near-field model predicts a discontinuous decrease over a more limited depth range. The two distributions could be brought into

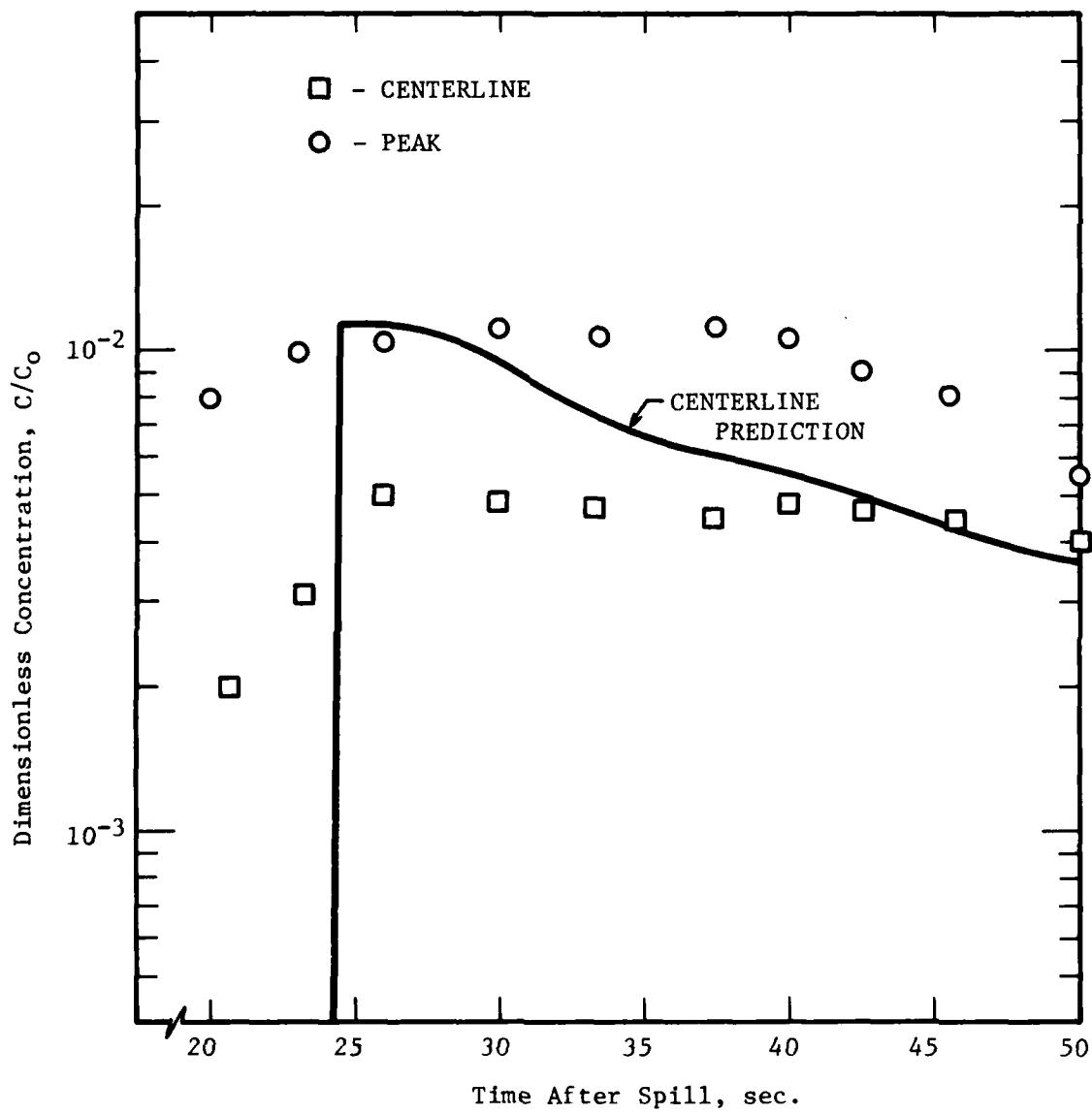


FIGURE V.22 CONCENTRATION VS. TIME AT
 $x = 5.03\text{m}$ (198 in.) AND
 $z = 0.235\text{m}$ (9.25 in.) FOR
SODIUM SILICATE, s.g. = 1.4

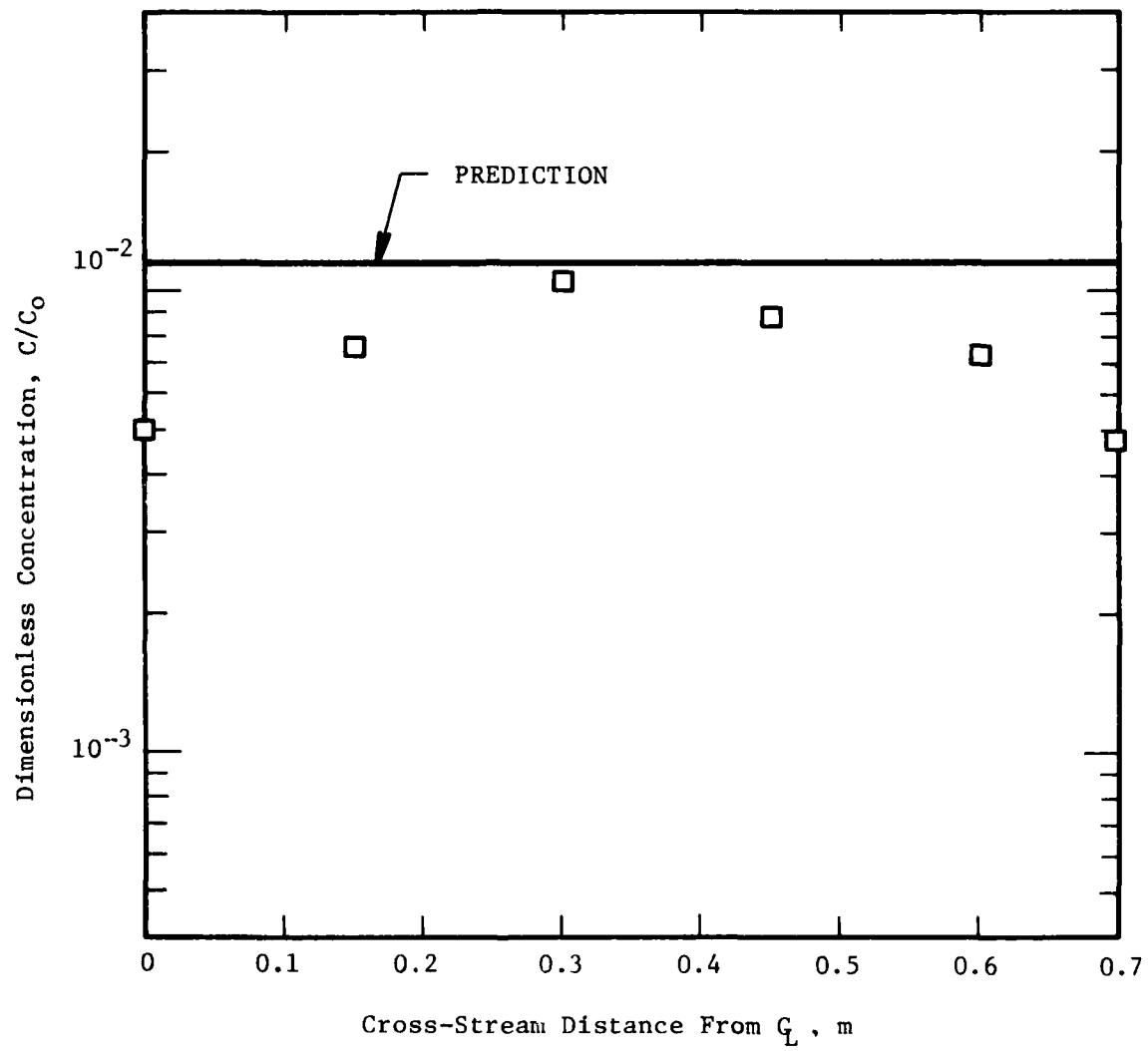


FIGURE V.23 CROSS-STREAM CONCENTRATION AT
 $x = 5.03\text{m}$ (198 in.),
 $z = 0.235$ (9.25 in.), AND
 $t = 26$ seconds FOR
SODIUM SILICATE, s.g. = 1.4

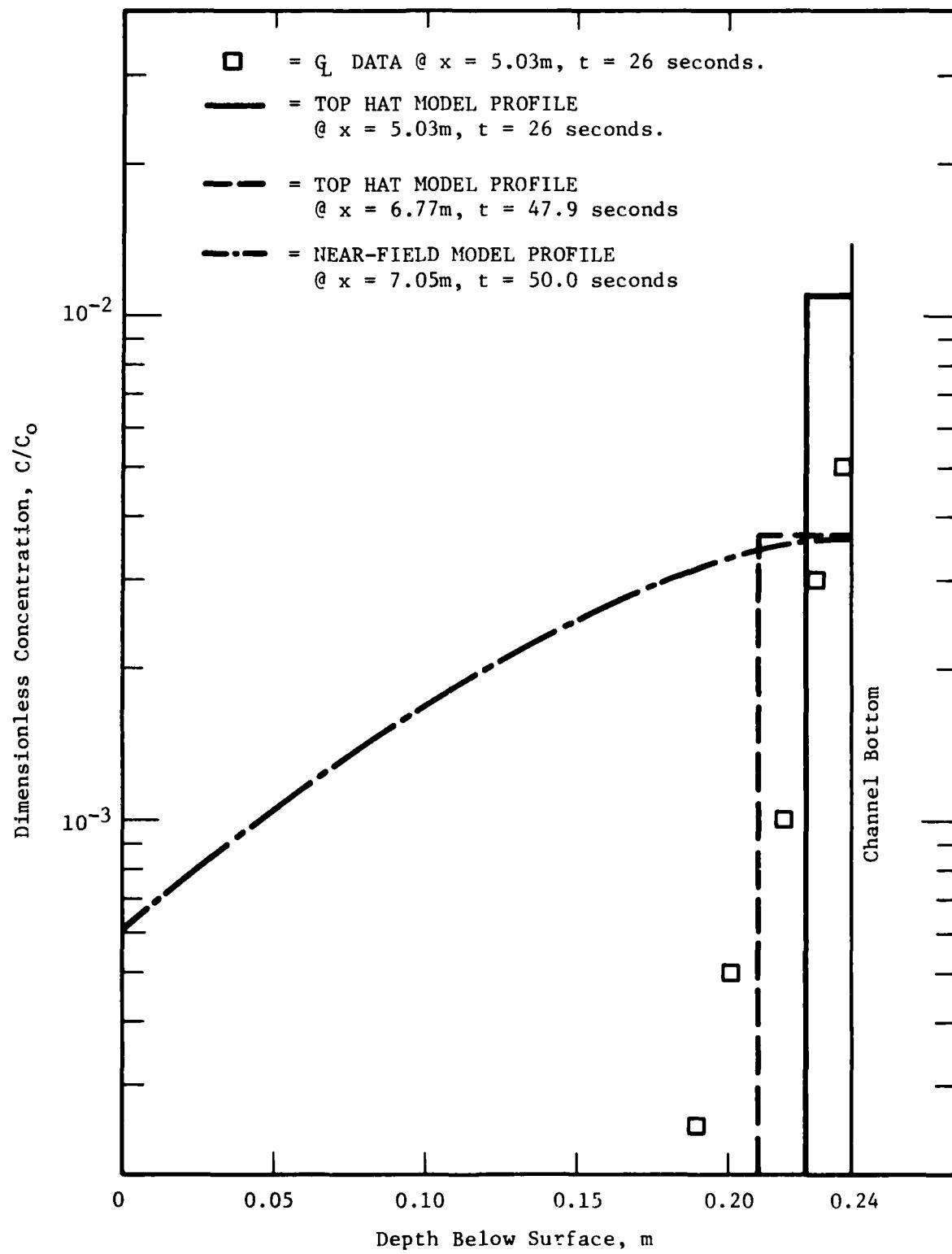


FIGURE V.24 CONCENTRATION VS. DEPTH FOR SODIUM SILICATE,
s.g. = 1.4

closer agreement by increasing the number of point sources (five) used in the near-field model to represent the cloud width. But somewhat further downstream the predictions would be unchanged, so five point sources are probably adequate. It might be noted that with $\epsilon_x = \epsilon_y$ the near-field concentration was predicted to be nearly uniform across the depth at the matching point; this is an independent verification that $\epsilon_x > \epsilon_y$.

Figures V.25 and V.26 compare the model to a spill of ethanol, s.g. = 0.79, which is strongly positively-buoyant. (Case II.1-2; mass spilled = 0.79 kg; spill location $z = d/2 = 0.114$ m; channel velocity = 0.141 m/sec.) The spill was shown pictorially in Figure IV.25. Centerline concentrations as a function of time are shown in Figure V.25. Again, the model predicts that the measurement location is in the very-near-field regime. The leading edge of the cloud is predicted to arrive about ten seconds or so ahead of the most concentrated part of the actual spill. Further adjustments of the empirical constants in the model, particularly to the denominator of the entrainment correlation (Equation (III.58b)), would decrease this apparent discrepancy in arrival times, but doing so would change the comparisons of the negatively-buoyant spill shown in Figure V.22. In fact, the constants were selected to give the best overall fit for all the tests, rather than for either Test II.1-14 or II.1-2 individually.

Comparisons of the predictions across the channel depth are shown in Figure V.26; the matching of the very-near-field and near-field models is also compared. Again, the comparisons are satisfactory. Note that buoyancy-induced mixing ends considerably sooner for this spill than for the negatively-buoyant spill discussed previously, even though both spills had the same volume.

The spill of a weakly negatively-buoyant chemical, s.g. = 1.05, is shown in Figures V.27 and V.28. (Case II.1-8B; spilled mass = 0.95 kg; spill location $z - d/2 = 0.114$ m; channel velocity = 0.141 m/sec.) The spilled volume is identical to the three cases discussed above. Buoyancy-induced mixing is predicted to end after about 15 seconds, and the test measurements thus are predicted to correspond to the turbulent-diffusion,

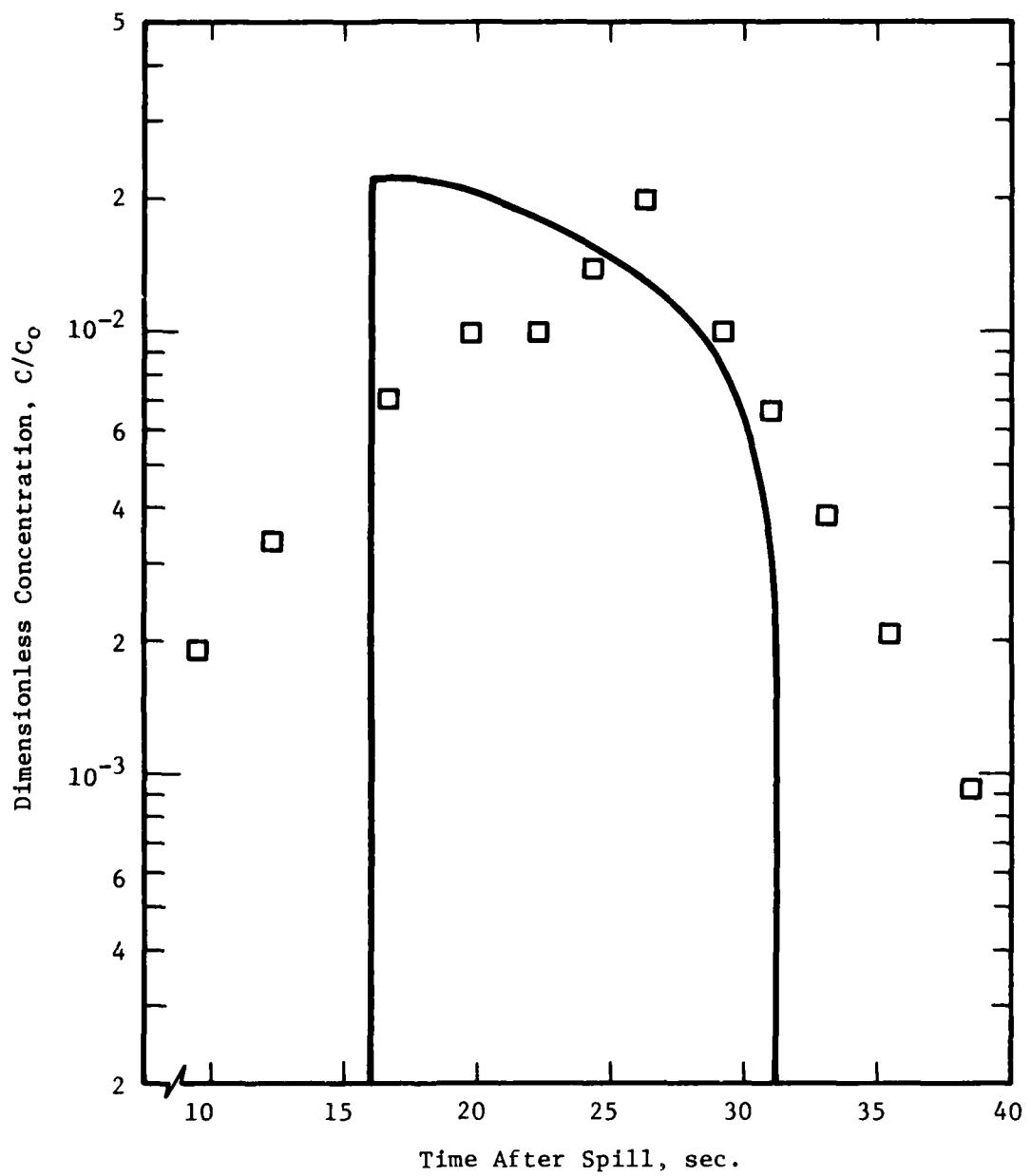


FIGURE V.25 CONCENTRATION VS. TIME AT
 $x = 3.57\text{m}$ (140 in.) AND
 $z = 0.0064\text{m}$ (0.016 in.)
FOR ETHANOL, s.g. = 0.79

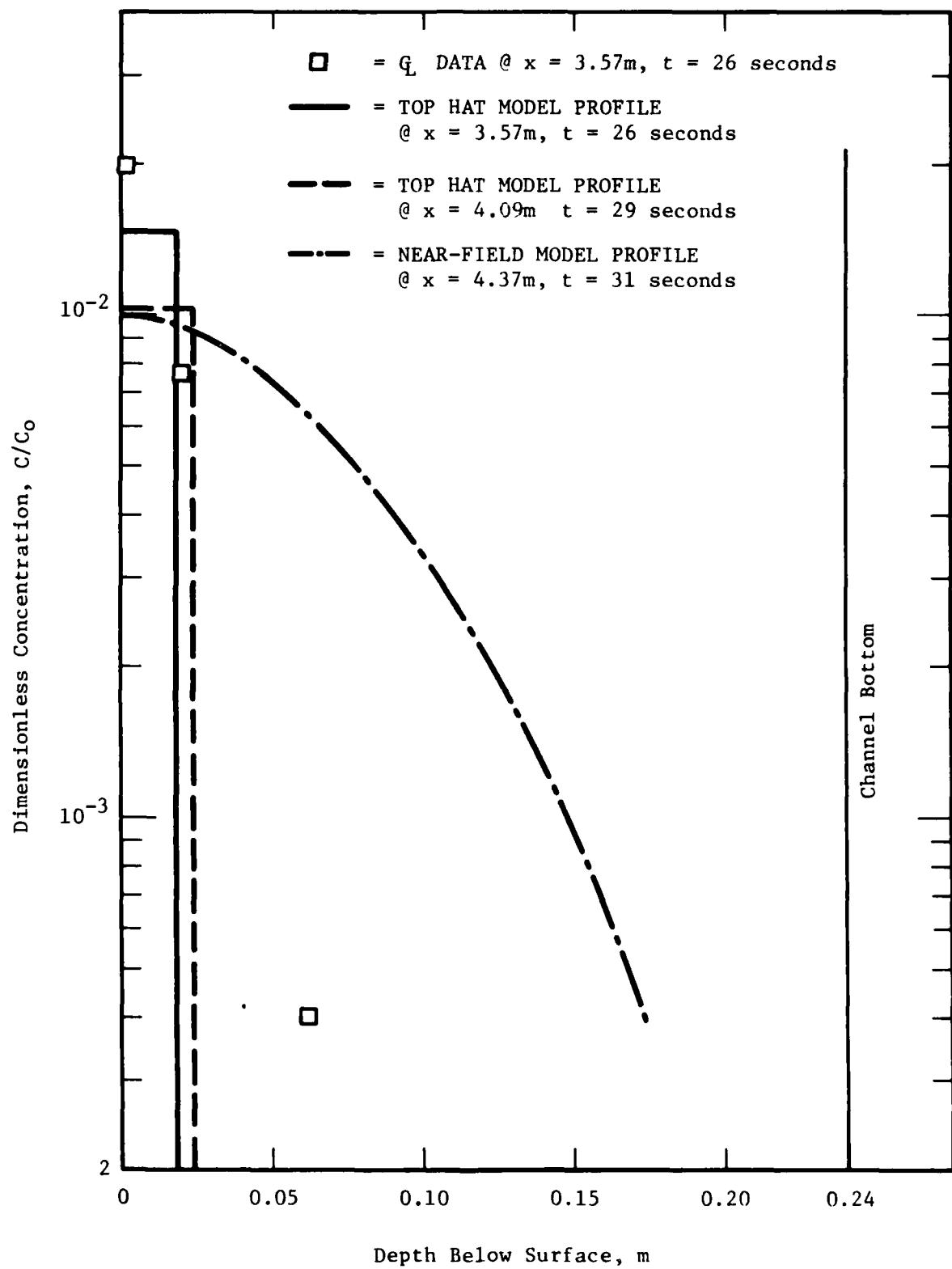


FIGURE V.26 CONCENTRATION VS. DEPTH FOR ETHANOL, s.g. = 0.79

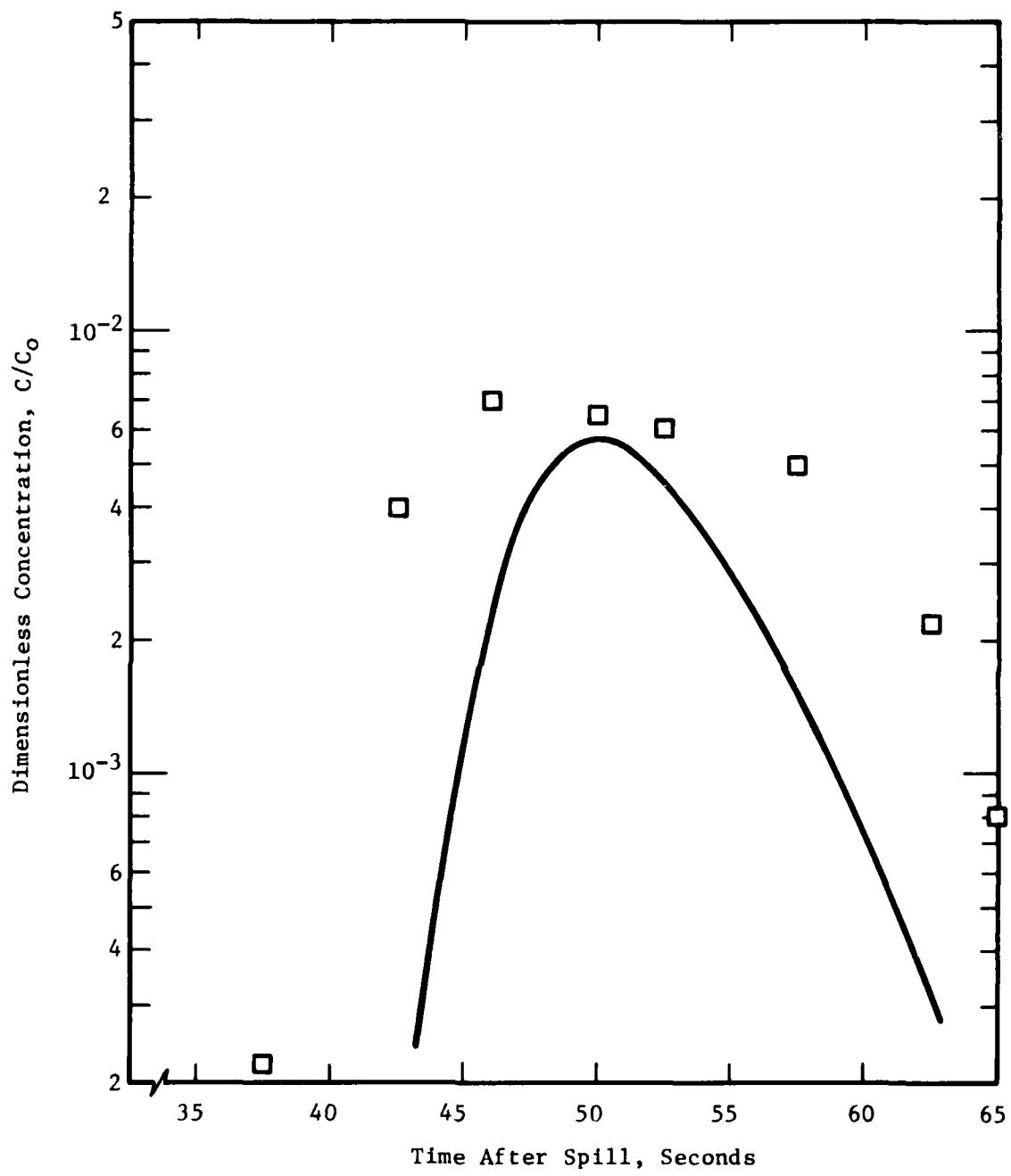


FIGURE V.27 CONCENTRATION VS. TIME AT
 $x = 7.08\text{m}$ (278 in.) AND
 $z = 0.235\text{m}$ (9.25 in.) FOR
SUGAR WATER, s.g. = 1.05

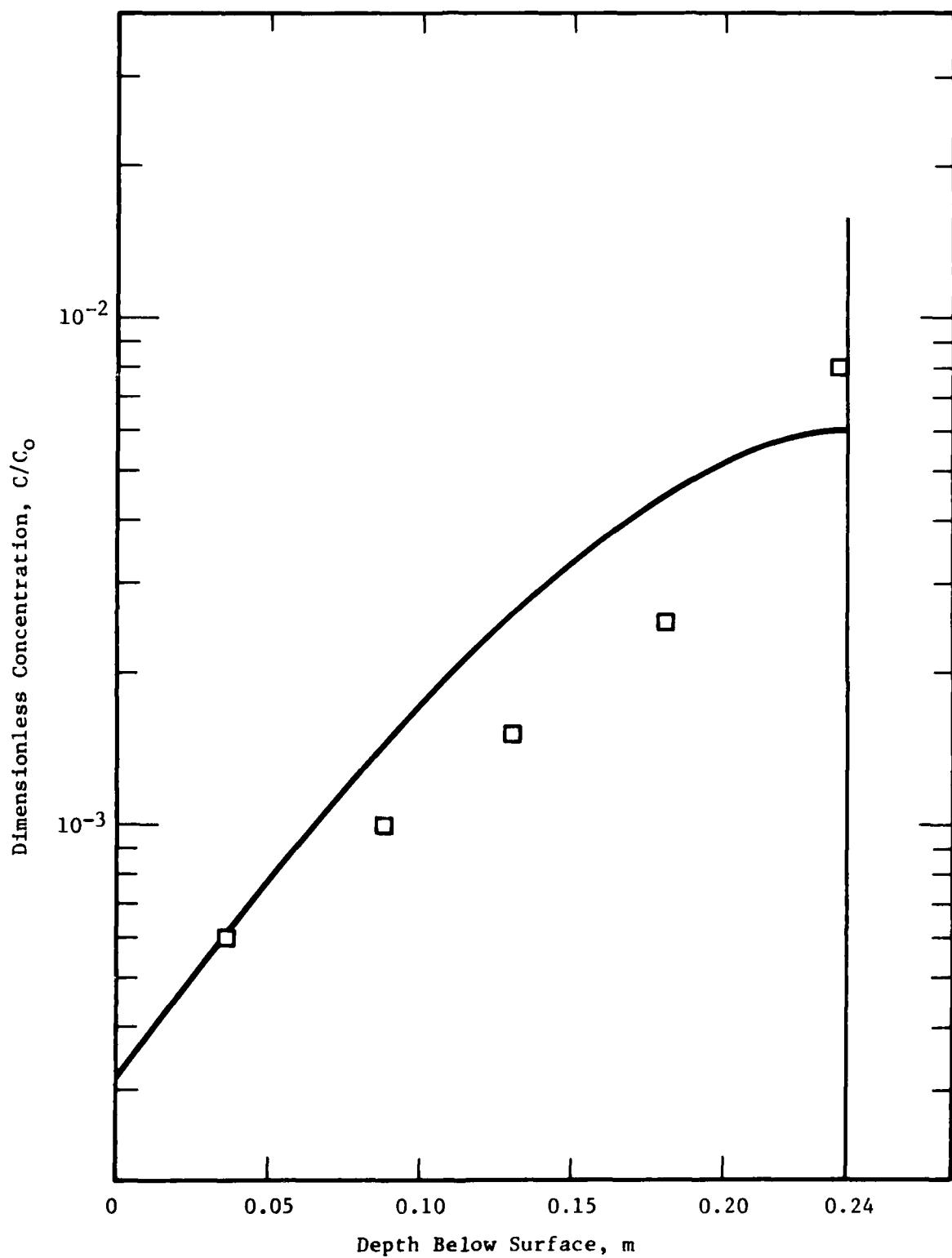


FIGURE V.28 CONCENTRATION VS. DEPTH AT
 $x = 7.08\text{m}$ (278 in.), $z = 0.235\text{m}$ (9.25 in.)
and $t = 50$ seconds FOR
SUGAR WATER, s.g. = 1.05

near-field regime, in contrast to the other two buoyant spills discussed above. As can be seen in the data of Figure V.27, the measured concentrations do rise and fall more gradually than for the previous cases and therefore indicate that diffusion is, in fact, an important dilution mechanism. The near-field model is in reasonably good agreement with the data, although the total duration of the affected region is underestimated somewhat. Figure V.28 gives comparisons of the concentration across the channel depth. It is evident that the test cloud has diffused significantly throughout the depth, which constitutes another confirmation of the model; the model predictions themselves also agree well with the data. Further, these near-field predictions depend implicitly on the very-near-field model. Thus, if the very-near-field dilution or time duration had been predicted poorly, the near-field model would not agree as well as it does with the test data.

Comparisons of other tests and the models are, in general, about as close as the four typical cases discussed above.

VI. CONCLUSIONS

The mixing, dilution, and evaporation models for water soluble chemicals previously developed by others for the Hazard Assessment Computer System (HACS) have been completely reformulated. The revised models now cover nearly every practical combination of spill density, spilling rate, total mass spilled, and type of waterway. In summary, there are now four models that can be used to assess the chemical concentration in the water from an accidental tank rupture:

1. A continuous spill in a steady river.
2. An instantaneous spill in a steady or a tidal river.
3. A continuous spill in a tidal river.
4. A continuous spill in an estuary or other coastal waters.

Only the first three models have been developed in detail as part of this program; the fourth model is already available as the "Dynamic Estuary Model."

Most of the program efforts were devoted to formulating better methods of predicting the chemical concentrations near the spill site, where the hazards are greatest. The previous HACS models used to compute these close-in concentrations, which were crude and unrealistic, would not have agreed with test data within an order of magnitude. Farther downstream from the spill site, in the "intermediate" and "far" fields, the new models and the previous ones are similar in form; the errors in the previous models have been corrected, however, and techniques have been developed to insure that the chemical concentration varies continuously rather than discontinuously when it is necessary to switch from a model appropriate to one dominant form of dilution to another.

For the first model, a continuous spill in a steady river, the mixing and dilution predictions now include:

- o the effects of the momentum and buoyancy of the chemical stream discharged from the punctured tank on the trajectory and dilution (entrainment of water) of the chemical plume;

- o the buoyancy-induced cross-stream spreading of the plume after it reaches either the upper or lower surface of the river;
- o the effect of density stratification between the plume and the water on the rate of entrainment;
- o a more accurate accounting of the waterway boundaries on the dilution processes; and
- o evaporation of chemical vapor from a plume at the water surface.

The model is based partially on previous work related to heavy-gas plumes near the surface of the ground.

The model of an instantaneous spill in a steady or tidal river now includes:

- o the buoyancy-induced spreading and dilution of the spilled volume after it reaches the upper or lower surface of the river;
- o the effect of density stratification between the cloud of chemical and the water on the rate of entrainment;
- o a more accurate accounting of the waterway boundaries on the dilution processes;
- o evaporation of vapor from a chemical cloud at the water surface; and
- o the transient effects of a tidal flow on all the important dilution mechanisms.

The prediction methods are based partially on previous well-verified models of the dilution of heavy-gas clouds near the surface of the ground.

The third model, a continuous spill in a tidal river, includes many of the effects listed above for a spill in a steady river. However, because of analytical difficulties, buoyancy-induced cross-stream spreading in a transient flow could not be included; thus, this model does not predict the close-in concentrations of buoyant chemicals as well as the steady-river model does. The model does include the effects of the tidal current on all the other dilution mechanisms, as well as the possibility that the river water may pass back-and-forth through the spill site several times.

The predictions of the continuous and instantaneous spill models for a steady river, in the close-in or near-field range, were compared to scale-model tests conducted over a wide range of discharge rates and volumes, river speeds, and chemical densities. (Lack of a suitable test facility prevented a verification of the tidal river models.) Part of the test data was used to determine "best" values of the empirical constants in the models. The remaining tests were then used to verify the revised models. In all cases, a generally close comparison of the model predictions and the test results was found.

It is concluded, then, that the revised mixing and dilution models for water soluble chemicals are now suitable for inclusion in the Hazard Assessment Computer System.

VII. REFERENCES

1. P. P. K. Raj and A. S. Kalekar, "Assessment Models in Support of the Hazard Assessment Handbook," Report CG-D-65-74, Arthur D. Little, Inc., Cambridge, Mass., 1974. (NTIS Report No. AD 776-617).
2. N. A. Eisenberg, C. J. Lynch, R. M. Kumar, R. J. Bredina, and M. N. Durrani, "A Critical Technical Review of Six Hazard Assessment Models," Report CG-D-122-76, Enviro Control, Inc., Rockville, Md., 1975. (NTIS Report No. AD A035-599).
3. G. Ooms, "A New Method for the Calculation of the Plume Path of Gases Emitted by a Stack," Atmospheric Environment, Vol. 6, pp. 899-909, 1972.
4. G. W. Colenbrander, "A Mathematical Model for the Transient Behavior of Dense Vapor Clouds," 3rd International Symposium on Loss Prevention and Safety Promotion in the Process Industries, 1980.
5. H. B. Fischer, E. J. List, R. C. Y. Koh, J. Imberger, and N. H. Brooks, Mixing in Inland and Coastal Waters, Academic Press, 1979.
6. F. T. Dodge, E. B. Bowles, J. E. Mann, and R. E. White, "Experimental Verification and Revision of the Venting Rate Model of the Hazard Assessment Computer System and the Vulnerability Model," Final Report, U. S. Coast Guard Contract DOT-CG-73623-A, July 1980.
7. F. T. Dodge and E. B. Bowles, "Draining of Tanks With Submerged Outlets or Without Vacuum-Relief," Trans. ASME, Journal of Fluids Engineering, Vol. 104, pp. 67-71, March 1982.
8. D. B. Turner, "Atmospheric Dispersion Modeling, A Critical Review," Journal of the Air Pollution Control Association, Vol. 29, No. 5, 1979.
9. G. A. Briggs, "Plume Rise Predictions," Chapter 3 in Lectures on Air Pollution and Environmental Impact Analysis, D. A. Haugen, editor, American Meteorological Society, Boston 1975.
10. T. B. Morrow, F. T. Dodge, E. B. Bowles, and W. J. Astleford, "Mixing and Dilution of Water Soluble Hazardous Chemicals Released in Navigable Rivers," ASME Paper 81-FE-17, 1981.
11. H. Rouse and J. Howe, Basic Mechanics of Fluids, John Wiley and Sons, 1953.
12. Anon., "Estimating Aquatic Dispersion of Effluents from Accidental and Routine Reactor Releases for the Purpose of Implementing Appendix I," U. S. Nuclear Regulatory Commission Regulatory Guide 1.113, April 1977.
13. H. Liu, "Predicting Dispercient Coefficient of Streams," Proc. ASCE, J. Environmental Engrg. Div., Vol. 103, pp. 59-69, Feb. 19771

14. K. J. Eidsvik, "A Model for Heavy Gas Dispersion in the Atmosphere," Atmospheric Environment, Vol. 14, pp. 769-777, 1980.
15. J. A. Havens, "A Review of Mathematical Models for Prediction of Heavy Gas Atmospheric Dispersion," I. Chem. E. Symposium Series No. 71, pp. 1-24, 1981.
16. R. Smith, "Contaminant Dispersion in Oscillatory Flows," J. Fluid Mech., Vol. 114, pp. 379-398, 1982.
17. K. D. Feigner and S. H. Harrison, "Documentation Report: FWQA Dynamic Estuary Model," U. S. Department of the Interior, Washington, D.C., July 1970.
18. L. J. Thibodeaux, "Mechanisms and Idealized Dissolution Modes for High Density ($p > 1$), Immiscible Chemicals Spilled in Flowing Aqueous Environments," AIChE Journal, Vol. 23, No. 4, July 1977.
19. S. J. Wright, "Effects of Ambient Crossflows and Density Stratification on the Characteristic Behavior of Round, Turbulent Buoyant Jets," Ph.D. Thesis, California Institute of Technology, Dept. of Civil Engineering, 1977. Available from Xerox University Microfilms, #77-22,330.
20. D. Mackay and T. K. Yuen, "Volatilization Rates of Organic Contaminants from Rivers," Water Poll. Res. J. of Canada, Vol. 15, pp. 83-98, 1980.

APPENDIX A

FURTHER DETAILS OF MODELS FOR
CONTINUOUS SPILLS IN STEADY RIVERS

FURTHER DETAILS OF MODELS FOR
CONTINUOUS SPILLS IN STEADY RIVERS

The computing equations given for the near-, intermediate-, and far-field concentrations for observation times after the spill has ceased can be derived by integrating the effects of a stream of corresponding instantaneous spills. For example, the near-field concentration is:

$$C(x, y, z, t) = \int_0^{t_e} \left\{ \frac{\dot{M} d\tau e^{-[x-u(t-\tau)]^2/4\varepsilon_x(t-\tau)}}{[4\pi(t-\tau)]^{3/2} (\varepsilon_x \varepsilon_y \varepsilon_z)^{1/2}} \right\} \times \sum_{n=1}^5 \exp \left[-(y-y_n)^2/4\varepsilon_y(t-\tau) - (z-z_n)^2/4\varepsilon_z(t-\tau) \right] \quad (A.1)$$

Here, the strength of the instantaneous spill is $\dot{M}d\tau$ and τ is the time at which each spill is inserted into the water. Equation (A.1) can be integrated in terms of error functions by making the substitutions

$$\xi = (t - \tau)^{-1/2} \quad (A.2a)$$

and

$$R_n^2 = x^2 + \frac{\varepsilon_x}{\varepsilon_y} (y - y_n)^2 + \frac{\varepsilon_x}{\varepsilon_z} (z - z_n)^2 \quad (A.2b)$$

This gives:

$$C(x, y, z, t) = \int_{\frac{1}{\sqrt{t}}}^{\frac{1}{\sqrt{t-t_e}}} \left\{ \left[\frac{2 \dot{M} d\xi}{(4\pi)^{3/2} (\varepsilon_x \varepsilon_y \varepsilon_z)^{1/2}} \right] [\exp(xu/z\varepsilon_x)] \right\} \times \sum_{n=1}^5 \exp \left[-u^2/4\varepsilon_x \xi^2 - R_n^2 \xi^2/4\varepsilon_x \right] \quad (A.3)$$

The integration gives Equation (III.44) of Section III.2.5. Incidentally, if $t_e \rightarrow \infty$ the steady-stage solution, Equation (III.27) of Section III.2.4, is obtained; the same result is also obtained for finite t_e if ϵ_x is small and $x < ut \leq u t_e$ (i.e., the observation point is within the spill and the spill has not yet ceased).

Equation (III.45) for the intermediate field is obtained by integrating a stream of instantaneous line sources:

$$C(x, y, t) = \int_0^{t_e} \left\{ \frac{\dot{M} d\tau}{[4\pi e_x(t-\tau)]^{1/2} w d} \right\} \exp \left\{ -\frac{[x-u(t-\tau)]^2}{4 e_x(t-\tau)} \right\} \times \\ \left\{ 1 + 2 \sum_{m=1}^{\infty} \cos \frac{m\pi w_s}{w} \cos \frac{m\pi(y+w/2)}{w} \exp \left[\frac{-m^2\pi^2 e_y(t-\tau)}{w^2} \right] \right\} \quad (A.4)$$

The necessary substitutions are

$$\xi = (t-\tau)^{1/2} \quad (A.5a)$$

and

$$\omega_m^2 = m^2\pi^2 e_y/w^2 \quad (A.5b)$$

Equation (III.48) for the far-field can be found similarly:

$$C(x, t) = \int_0^{t_e} \left\{ \frac{\dot{M} d\tau}{w d [4\pi E_x(t-\tau)]^{1/2}} \right\} \exp \left\{ -\frac{[x-u(t-\tau)]^2}{4 E_x(t-\tau)} \right\} \quad (A.6)$$

The necessary substitution to get an integrable form is:

$$\xi = (t-\tau)^{1/2} \quad (A.7)$$

APPENDIX B

FURTHER DETAILS OF INSTANTANEOUS SPILL
MODELS FOR STEADY AND TIDAL RIVERS

FURTHER DETAILS OF INSTANTANEOUS SPILL
MODELS FOR STEADY AND TIDAL RIVERS

B.1 Evaporation Model

Evaporation from the very-near-field region of lighter-than-water chemical spills is computed by the model suggested by Mackay and Yuen [20]:

$$\frac{dm_e}{dt} = HC \quad (B.1)$$

Here, m_e is the evaporated mass per unit area of surface and H is an evaporation mass transfer coefficient. Equation (B.1) assumes that concentration of chemical in the air is negligible.

H is equal to $1/R_T$, where R_T is the total resistance to evaporation, a combination of R_1 , the resistance to diffusion from the chemical in the river to the near surface water, R_2 , the resistance to diffusion through the near surface liquid to the interface, and R_3 , the resistance to diffusion of chemical through the layer of air close to the water surface. R_1 is negligibly small for a highly concentrated cloud at the surface. R_2 varies somewhat with each specific case, but [20] recommends a typical value of 2.5×10^4 sec/meter. R_3 depends on both an air-water mass transfer coefficient, which for typical conditions is estimated to 0.01/meter/sec, and the equilibrium value of the concentration at the air-water interface; the total recommended value of R_3 is $2.4/\mathcal{H}$ sec/meter, where \mathcal{H} is Henry's constant in units of atm-m³/mole. For highly soluble chemicals, \mathcal{H} is of the order of 10^{-5} . Altogether, then, the evaporation mass transfer coefficient is typically:

$$H \approx [2.5 \times 10^4 + 2.4 \times 10^5]^{-1} = 3.8 \times 10^{-5} \text{ m/sec} \quad (B.2)$$

Because of the small value of \mathcal{H} for the chemicals of interest to the Coast Guard, the predicted evaporation rate will also be small ordinarily. It might be neglected, then, with little loss of accuracy.

B.2 Tidal Effects of e_x and the Intermediate Field

The very-near-field dilution is too rapid to be affected by the tides. In the near-field, the dilution is caused by turbulent diffusion, and this too is unaffected by the tidal flow if the diffusion coefficients are computed on the basis of an appropriate shear velocity. In the intermediate-field, longitudinal dispersion is, however, affected by the tidal flow; it will be shown below that both the dispersion coefficient and the form of the governing equation for dispersion must account for time-varying effects.

When the current has a velocity gradient and the concentration is fairly uniform across the depth (i.e., the intermediate-field), the chemical attempts to spread downstream at varying speeds across the depth. Diffusion, however, attempts to keep the concentration uniform across the depth. The net effect is a more rapid mixing by "dispersion" than by diffusion alone. As shown in [5], the general formula for the dispersion coefficient is

$$e_x = -\frac{1}{\varepsilon_z d} \int_0^d (u - \bar{u}) \int_0^z \int_0^z (u - \bar{u}) dz dz dz \quad (B.3)$$

where \bar{u} is the depth-averaged velocity; $u - \bar{u}$ is, thus, the velocity variation due to both the gradient and turbulent fluctuations. The concentration variation, $C - \bar{C}$, is given from the solution of the mass transfer balance [5] as:

$$C - \bar{C} = \frac{1}{\varepsilon_z} \left(\frac{\partial \bar{C}}{\partial x} \right) \int_0^z \int_0^z (u - \bar{u}) dz dz + (C - \bar{C}) \Big|_{z=0} \quad (B.4)$$

Equations (B.3) and (B.4) can be combined to give:

$$e_x = - [d(\partial \bar{C} / \partial x)]^{-1} \int_0^d (u - \bar{u}) (C - \bar{C}) dz \quad (B.5)$$

In order to evaluate Equation (B.5), a linear velocity gradient is assumed temporarily for the steady and the time-averaging parts of the tidal current. Equation (B.4) is used to determine the functional relation of $C - \bar{C}$, which is then inserted in Equation (B.5) and integrated to give:

$$e_x = \frac{(u_o - \bar{u}_o)^2 d^2}{120 \epsilon_z} + \frac{(u_1 - \bar{u}_1)^2 d^2 \bar{T}}{240 \epsilon_z} \left\{ 1 - \frac{1}{2} \cos \left[\frac{4\pi}{T} (t + \alpha) + \theta \right] \right\} \\ + \frac{(u_o - \bar{u}_o)(u_1 - \bar{u}_1) d^2}{480 \sqrt{2} \epsilon_z} \left\{ \bar{T} \sin \left[\frac{2\pi}{T} (t + \alpha) + \theta \right] + 4 \sin \left[\frac{2\pi}{T} (t + \alpha) \right] \right\} \quad (B.6)$$

Here $\bar{T} = (Td^2/\epsilon_z) [\pi^2/4 + (Td^2/\epsilon_z)^2]^{-1/2}$ and θ , is defined by Equation (III.70). A number of small higher-order terms have been neglected in Equation (B.6). In a river, the velocity gradient is not linear and there are also turbulent fluctuations. For a steady river, the use of the correct velocity profile would presumably give $5.93 du_*$, the empirical correlation, instead of $(u_o - \bar{u}_o)^2 d^2/120 \epsilon_z$ in Equation (B.6) for the time-independent part. Assuming the tidal velocity profile and turbulence level are the same as the steady component, $(u_1 - \bar{u}_1)^2 d^2/120 \epsilon_z$ should also be replaced by $5.93 du_*$. By making these substitutions and separating the constant and time-dependent parts of Equation (B.6), the expressions for e_x and e_t given as Equations (III.68) and (III.69) can be derived.

The intermediate-field concentration is determined by the balance between mass storage, diffusion, and dispersion [5]:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = (e_x + e_t) \frac{\partial^2 C}{\partial x^2} + \epsilon_y \frac{\partial^2 C}{\partial y^2} \quad (B.7)$$

This differential equation can be simplified by making the transformation

$$\zeta = x - \int_0^t u \times dt \quad \text{and} \quad \tau = t; \quad \text{Doing so gives:}$$

$$\frac{\partial C}{\partial \tau} = (e_x + e_t) \frac{\partial^2 C}{\partial \zeta^2} + \epsilon_y \frac{\partial^2 C}{\partial y^2} \quad (B.8)$$

A solution of the form

$$C = C_0 + \sum_{n=1}^{\infty} \left(\frac{e_t}{e_x} \right)^n C_n \quad (B.9)$$

will be sought; note that $|e_t| \leq e_x$, so the series should converge. Substituting Equation (B.9) into Equation (B.8), and collecting powers of (e_t/e_x) gives the following set of differential equations:

$$\frac{\partial C_0}{\partial \tau} = e_x \frac{\partial^2 C_0}{\partial \zeta^2} + \epsilon_y \frac{\partial^2 C_0}{\partial y^2} \quad (B.10a)$$

$$\frac{\partial C_1}{\partial \tau} + \left(\frac{\dot{e}_t}{e_t} \right) C_1 = e_x \frac{\partial^2 C_0}{\partial \zeta^2} + e_x \frac{\partial^2 C_1}{\partial \zeta^2} + \epsilon_y \frac{\partial^2 C_1}{\partial y^2} \quad (B.10b)$$

•
•
•
•

The steady line-source solution of Equation (B.10a) for the appropriate initial and boundary conditions is given in [12] as:

$$C_0 = \frac{M}{w d (4\pi e_x \tau)^{1/2}} \left[\exp \left(-\zeta^2 / 4e_x \tau \right) \right] \times$$

$$\left\{ 1 + 2 \sum_{m=1}^{\infty} \cos \frac{m\pi w_s}{w} \cos \left[\frac{m\pi (y + w/2)}{w} \right] \exp \left[-\frac{m^2 \pi^2 \epsilon_y \tau}{w^2} \right] \right\} \quad (B.11)$$

A solution of Equation (B.10b) that satisfies all the initial and boundary conditions for $C - C_o$ is:

$$C_1 = -\frac{\zeta}{2} \left(\frac{\partial C_o}{\partial \zeta} \right) + \phi_1 \quad (B.12)$$

Here, ϕ_1 is a correction term that is the solution of a differential equation derived by substituting Equation (B.12) into (B.10b) and collecting terms. This "correction" differential equation is of the same form as Equation (A.10b) but the $e_x(\partial^2 C_o / \partial \zeta^2)$ on the right is replaced by $-\zeta \dot{e}_t (\partial C_o / \partial \zeta) / 2 e_t$. Now, $\dot{e}_t \zeta (\partial C_o / \partial \zeta) / 2 e_t$ is much smaller in magnitude than $e_x(\partial^2 C_o / \partial \zeta^2)$ as a direct comparison will show. Because of this much reduced "forcing" term, the magnitude of ϕ_1 is much smaller than C_1 ; in fact, both ϕ_1 and C_1 approach zero for $\zeta = 0$ and $\zeta \rightarrow \infty$, and are therefore both smaller than C_o . Neglecting all higher approximations in Equation (B.9), the line-source solution for a tidal river is:

$$\begin{aligned} C &= C_o \left[1 - \zeta \left(\frac{\partial C_o}{\partial \zeta} \right) / 2 C_o \right] \\ &= C_o \left[1 + (\zeta^2 / 4 e_{xt}) (e_t / e_x) \right] \end{aligned} \quad (B.13)$$

This is Equation (III.67) when the images are added.

A.3 Tidal Effects of E_x and the Far-Field

The same kind of analysis performed for e_x shows that E_x and E_t , the far-field dispersion coefficients, depend on the tidal component in exactly the same way as e_x and e_t .

The far-field model for a steady river is

$$C_o(x, t) = \left[\frac{M}{(4\pi E_x t)^{1/2} w d} \right] \exp(-\zeta^2 / 4E_x t) \quad (B.14)$$

It can be derived from Equation (B.11) by replacing e_x with E_x and by realizing that the minimum time for the validity of the far-field model is such that $\exp[-\pi^2 \epsilon_y t / w^2] \approx 0$. The tidal river form follows from Equation (B.13).

APPENDIX C

FURTHER DETAILS OF CONTINUOUS SPILL
MODELS FOR A TIDAL RIVER

FURTHER DETAILS OF CONTINUOUS SPILL
MODELS FOR A TIDAL RIVER

C.1 Deviation of Near-Field Model

As stated in Section III.4.2, the near-field model for a continuous spill is derived by integrating the effects of a stream of instantaneous point sources, each of strength $\dot{M}dt$. That is:

$$C(x, y, z, t) = \int_0^t \frac{\dot{M}d\tau \exp [-(x - \bar{u}\tau)^2 / 4\epsilon_x(t-\tau)]}{[4\pi/(t-\tau)]^{3/2} (\epsilon_x \epsilon_y \epsilon_z)^{1/2}} \times \sum_{n=1}^5 \exp \left[-(y - y_n)^2 / 4\epsilon_y(t-\tau) - (z - z_n)^2 / 4\epsilon_z(t-\tau) \right] \quad (C.1)$$

Here, $\bar{u}\tau = \int u * dt$; τ , the time at which the instantaneous source enters the water, τ varies from 0 to t , where t is the observation time, which does not vary in the integration; and the $(t - \tau)$ terms account for the fact that the sources do not all act from $t = 0$.

Equation (B.1) cannot be integrated exactly, because of the time-varying part of u . For a steady river, the integration is possible, and the result does not depend on ϵ_x ; see, for example, Equation (III.27). The lack of a dependency on ϵ_x is because backward and forward longitudinal diffusion exactly cancel. The cancellation will also occur approximately for a tidal river unless ϵ_x is very large or the river speed is very small. Put another way, the integrand in Equation (C.1) will make a contribution to the total concentration only for those values of x and t such that $(x - \bar{u}\tau)^2$ is less than $4\epsilon_x(t - \tau)$. Since for a steady river, the result is independent of ϵ_x , it is legitimate to take the limit $\epsilon_x \rightarrow 0$; in that case, the integrand is zero unless $x - \bar{u}\tau = 0$ identically.* (The answer when ϵ_x is not negligible will be derived later.) Consequently, only the point sources

* The same result for a steady river is obtained, in fact, by exact integration or by taking the limit $\epsilon_x \rightarrow 0$.

that are inserted at certain times τ_j will add up to give a net contribution at the observation point x at the observation time t ; these times are the roots of

$$x - \int_{\tau_j}^t u \times d\tau = 0 \quad (C.2a)$$

This is Equation (III.76). By making the transformation $\zeta(\tau) = x - \bar{u}t$, it can be seen that $d\xi = u(\tau) \times d\tau = u_\tau \times d\tau$, where u_τ is the value of u for $t = \tau$. Further, by defining a time-average velocity as

$$\bar{u} = \left[\int_{\tau}^t u \times d\tau \right] / (t - \tau), \quad (C.2b)$$

the observation point can be expressed as $x = \bar{u}(t - \tau_j)$.

Finally, according to the argument given above, the integrand is non-zero only for a vanishing small range around $\zeta = 0$ for each of the τ_j ; that is, the integral needs to be considered only for:

$$\tau_j - (\bar{\delta}/2 u_{\tau_j}) < \tau < \tau_j + (\bar{\delta}/2 u_{\tau_j}) \quad (C.3)$$

for all the τ_j , this range corresponds to $-\bar{\delta}/2 < \zeta < \bar{\delta}/2$ since $\zeta = 0$ for $\tau = \tau_j$. Hence, Equation (C.1) becomes:

$$C(x, y, z, t) = \lim_{\substack{\epsilon_x \rightarrow 0 \\ \zeta \rightarrow 0}} \sum_{j=1}^M \left\{ \int_{-\bar{\delta}/2}^{\bar{\delta}/2} \frac{\dot{M}d\zeta / u_{\tau_j}}{(4\pi x / u_j)^{3/2} (\epsilon_x \epsilon_y \epsilon_z)^{1/2}} \times \right. \\ \left[\exp \left(-\zeta^2 \bar{u}_j / 4\epsilon_x x \right) \right] \times \sum_{n=1}^5 \exp \left[-(y - y_n)^2 \bar{u}_j / 4\epsilon_y x \right. \\ \left. \left. - (z - z_n)^2 \bar{u}_j / 4\epsilon_z x \right] \right\} \quad (C.4)$$

The limit $\epsilon_x \rightarrow 0$ must be taken before $\bar{\delta} \rightarrow 0$. (Since $\bar{\delta}$ is small, the variation of \bar{u} and u_T with τ is neglected in Equation (C.4), and they have been replaced by their values \bar{u}_j and u_{Tj} at $\tau = \tau_j$.) The only part of Equation (C.4) that varies with ζ is the first exponential function, and its integral is:

$$\int_{-\bar{\delta}/2}^{\bar{\delta}/2} \exp \left[-\zeta^2 \bar{u}_j / 4\epsilon_x x \right] d\zeta = 2 \left(\frac{\pi x \epsilon_x}{\bar{u}_j} \right)^{1/2} \operatorname{erf} \left[\delta (\bar{u}_j / 4x \epsilon_x)^{1/2} / 2 \right] \quad (C.5)$$

As $\epsilon_x \rightarrow 0$, the value of the error function is ± 1 , depending on whether $\bar{\delta} > 0$. Since $\bar{\delta} > 0$ when $u_{Tj} > 0$, and vice versa, the value of ± 1 can always be assumed, if the absolute value of u_{Tj} is used in Equation (C.4). Combining Equations (C.4) and (C.5) gives:

$$C(x, y, z, t) = \sum_{j=1}^M \left\{ \frac{\dot{M} \bar{u}_j}{4\pi x (\epsilon_y \epsilon_z)^{1/2} |u_{Tj}|} \times \sum_{n=1}^5 \exp \left[-(y-y_n)^2 \bar{u}_j / 4x \epsilon_y - (z-z_n)^2 \bar{u}_j / 4x \epsilon_x \right] \right\} \quad (C.6)$$

This is Equation (III.75).

The result for the case when u_{Tj} is so small that longitudinal dispersion is not negligible will be derived now. Since $u_{Tj} \approx 0$, the transformation $\zeta = x - \bar{u}t$ gives $d\zeta = u_T dt \approx 0$ for $u_T = u_{Tj} \approx 0$. It is thus not legitimate to replace u_T by u_{Tj} in the integrand with $\bar{\delta} \rightarrow 0$, since the entire integrand is singular for that case. Instead, a definite value of $\bar{\delta}$ will be determined. First, a proper value of $\Delta\zeta \approx d\zeta$ will be found. By definition:

$$\Delta\zeta + \zeta_j = x - \int_{\tau_j + \Delta\tau}^t u \times dt \quad (C.7)$$

Since $u = u_{\tau_j} = 0$ and $\zeta_j = 0$ for $\tau = \tau_j$, Equation (C.7) can be expanded to give:

$$\Delta\zeta = \frac{\pi u_1}{T} (\Delta\tau)^2 \left[\cos \frac{2\pi}{T} (\tau_j + \alpha) + \frac{2\pi \Delta\tau}{3T} \sin \frac{2\pi}{T} (\tau_j + \alpha) + \dots \right] \quad (C.8)$$

Unless the cosine term is identically zero, the $\Delta\zeta$ change for a $\Delta\tau$ change in τ around $\tau = \tau_j$ is therefore:

$$\Delta\zeta = \left[\frac{\pi u_1}{T} \cos \frac{2\pi}{T} (\tau_j + \alpha) \right] (\Delta\tau)^2 \quad (C.9)$$

The integration variable will now be taken as $\Delta\tau$, which will vary over $\pm \delta/2$. The variable $\zeta = \zeta_j + \Delta\zeta = \Delta\zeta$ is related to $\Delta\tau$ by Equation (C.9). The integral is, therefore,

$$\begin{aligned} C(x, y, z, t) = & \sum_{j=1}^M \int_{-\delta/2}^{\delta/2} \frac{\frac{M}{\dot{M}} (\Delta\tau)}{\left(4\pi x/\bar{u}_j\right)^{\gamma_2} (\epsilon_x \epsilon_y \epsilon_z)^{\gamma_2}} \times \\ & \exp \left\{ -\pi^2 u_1^2 \bar{u}_j \left[\cos \frac{2\pi}{T} (\tau_j + \alpha) \right]^2 (\Delta\tau)^4 / 4x \epsilon_x T^2 \right\} \times \\ & \sum_{n=1}^5 \exp \left[-(y-y_n)^2 \bar{u}_j / 4\epsilon_y x - (z-z_n)^2 \bar{u}_j / 4\epsilon_z x \right] \quad (C.10) \end{aligned}$$

Once again, the variation of \bar{u} over the small $\Delta\tau$ range has been neglected, so \bar{u} has been replaced by its value u_{τ_j} at $\tau = \tau_j$. A value for $\bar{\delta}$ can be determined by noting that the exponential term rapidly goes to zero as $\Delta\tau$ increases from zero. In fact, $\exp(-7) \approx 0.001$, so little is lost in the way of accuracy if the maximum value of $\Delta\tau = \bar{\delta}/2$ over which the integration is taken is chosen as:

$$\frac{\pi^2 u_1^2 \bar{u}_j \left[\cos \frac{2\pi}{T} (\tau_j + \alpha) \right]^2 (\bar{\delta}/2)^4}{4x \epsilon_x T^2} = 7 \quad (C.11)$$

Finally, since $\exp(-v) = 1 - v + v^2/v - \dots$, the integral can be evaluated for this value of $\Delta\tau$ to give:

$$C(x, y, z, t) = \sum_{j=1}^M \frac{2.6 \dot{M}^{1/2} \bar{u}_j^{5/4}}{(4\pi)^{1/2} (4\pi\epsilon_y\epsilon_z)^{1/2} \epsilon_x^{1/4} x^{5/4} u_1^{1/2} \left[\cos 2\pi/T (\tau_j + \alpha) \right]^{1/2}} \\ \times \sum_{n=1}^5 \exp \left[-(y-y_n)^2 \bar{u}_j / 4x\epsilon_y - (z-z_n)^2 \bar{u}_j / 4x\epsilon_z \right] \quad (C.12)$$

When $\cos \frac{2\pi}{T} (\tau_j + \alpha) = 0$, Equation (C.8) shows that

$$\Delta\zeta = \frac{2}{3} \left[\frac{\pi^2 u_1}{T^2} \sin \frac{2\pi}{T} (\tau_j + \alpha) \right] (\Delta\tau)^3 \quad (C.13)$$

Following through the same steps again shows that the leading term in Equation (C.12) is now

$$\frac{1.86 \dot{M}^{2/3} \bar{u}_j^{4/3}}{4\pi (4\pi\epsilon_y\epsilon_z)^{1/2} \epsilon_x^{1/6} x^{4/3} u_1^{1/3} \left[\sin 2\pi/T (\tau_j + \alpha) \right]^{1/3}}$$

These are the expressions given in Section III.4.2.

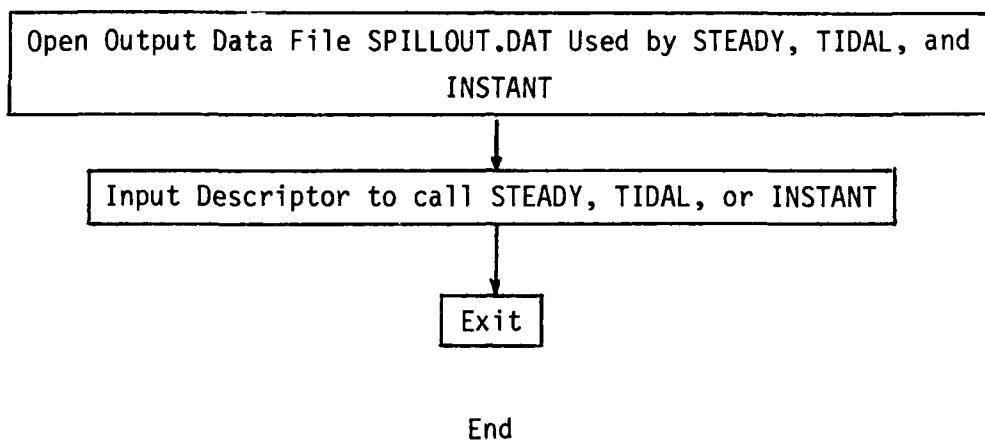
C.2 Derivation of Intermediate- and Far-Field Models

The derivation of these models follows exactly the same procedure as for the near-field model. Instead of using point-source solutions to form the integral, however, line-source and far-field instantaneous solutions are used. Note that only the "steady-river" term, as defined in Appendix A, make a contribution, since $\zeta = x - \bar{ut} = 0$ in the integrals, so the correction terms for the unsteady part disappear.

APPENDIX D

COMPUTER PROGRAM FLOW CHARTS

FIGURE D.1 FLOW CHART FOR PROGRAM "SPILL"



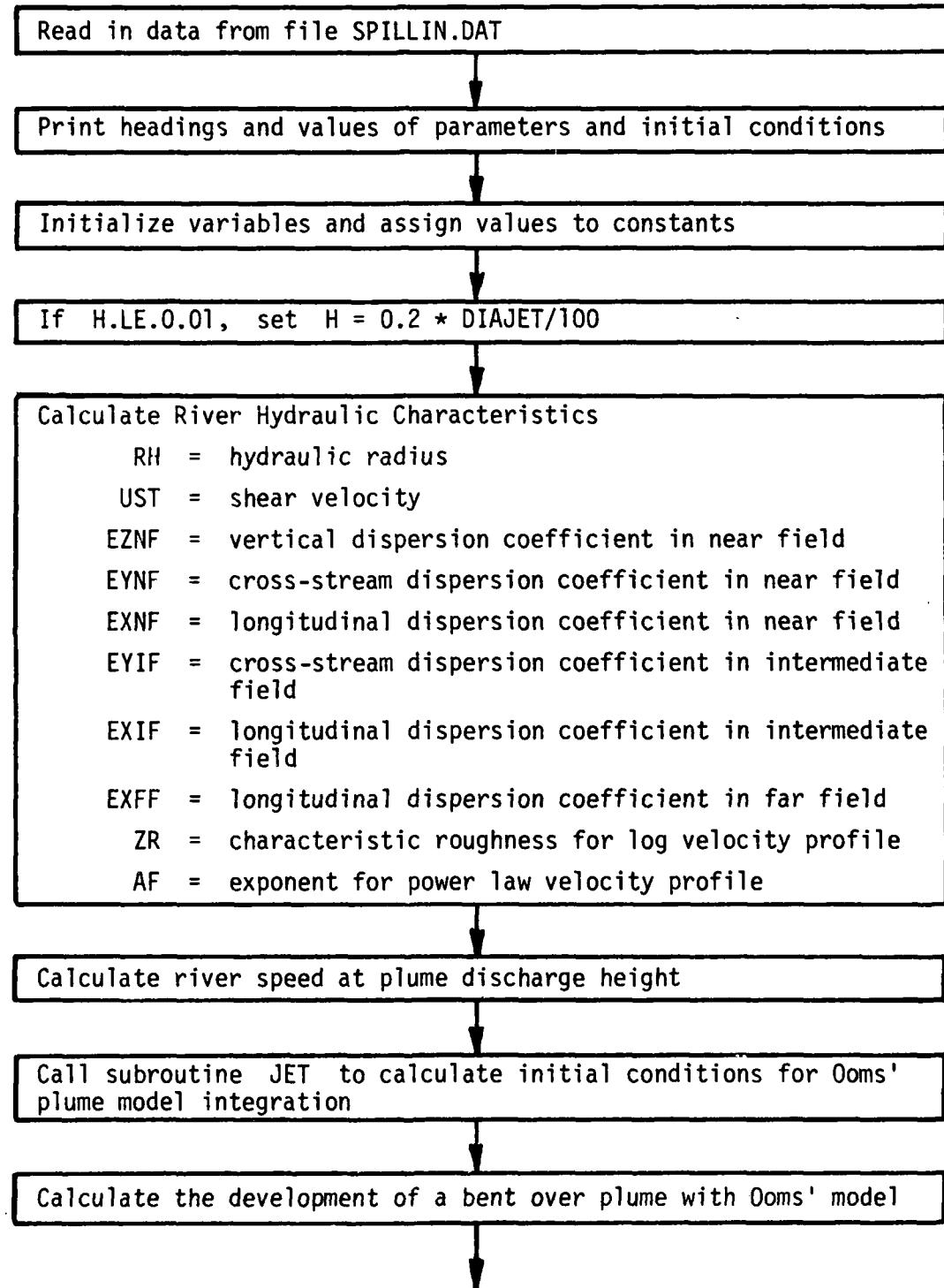
SUBROUTINE "JET"

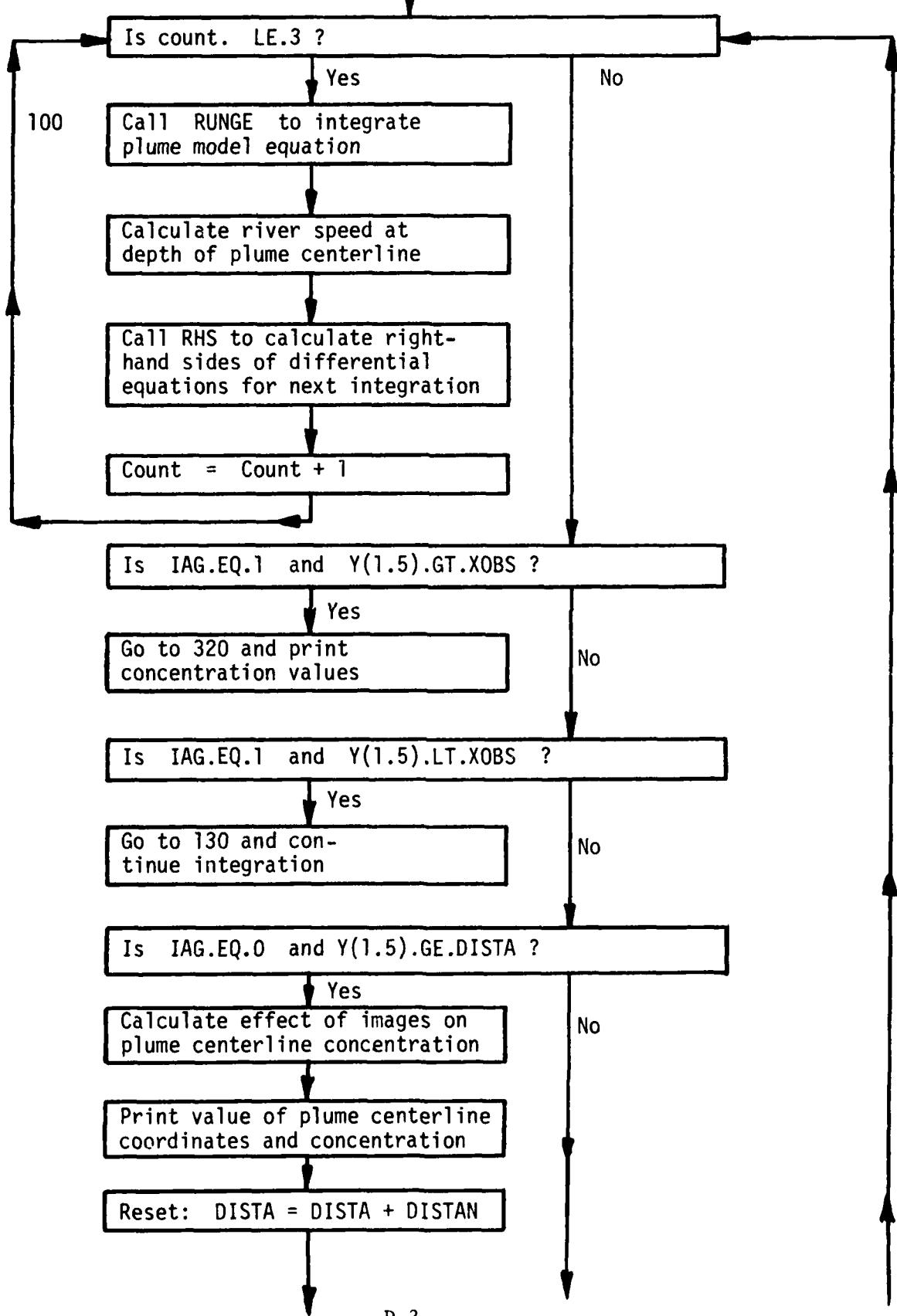
Transforms the initial tophat velocity profile of a continuous discharge to the Gaussian form needed by Ooms' model. Computes the deflection of the jet by the river during this period, a new jet diameter (because of the altered velocity profile), and the new virtual origin of the jet. (Uses empirical data from Kamotani and Greber to make the calculations.) Called by TIDAL and STEADY

SUBROUTINE "COEF"

Calculates ϵ_x , ϵ_y , ϵ_z , e_x , and E_x for a steady river and the time average part of e_x and E_x for a tidal river. Assumes that the roughness factor is $0.009 (m)^{1/6}$ for a laboratory channel and $0.025 (m)^{1/6}$ for a river. Called by TIDAL and STEADY

FIGURE D.2 FLOW CHART FOR PROGRAM "STEADY"





130

Is the plume centerline above the channel floor ?

Yes

No

Calculate Froude Number

Yes

Is Froude.LT.0 ?

No

Yes

Is Froude.GT.25. ?

No

Gravity spreading is possible,
Go to 200

131

Is the plume centerline below the channel surface?

Yes

No

Calculate Froude number

Yes

Is Froude.GT.0. ?

No

Yes

Is Froude.LT. - 25 ?

No

Gravity spreading is possible,
Go to 200

132

Is the plume diameter larger than the channel depth
or the channel width ?

Yes

Go to 300

No

Is the plume concentration very dilute ?

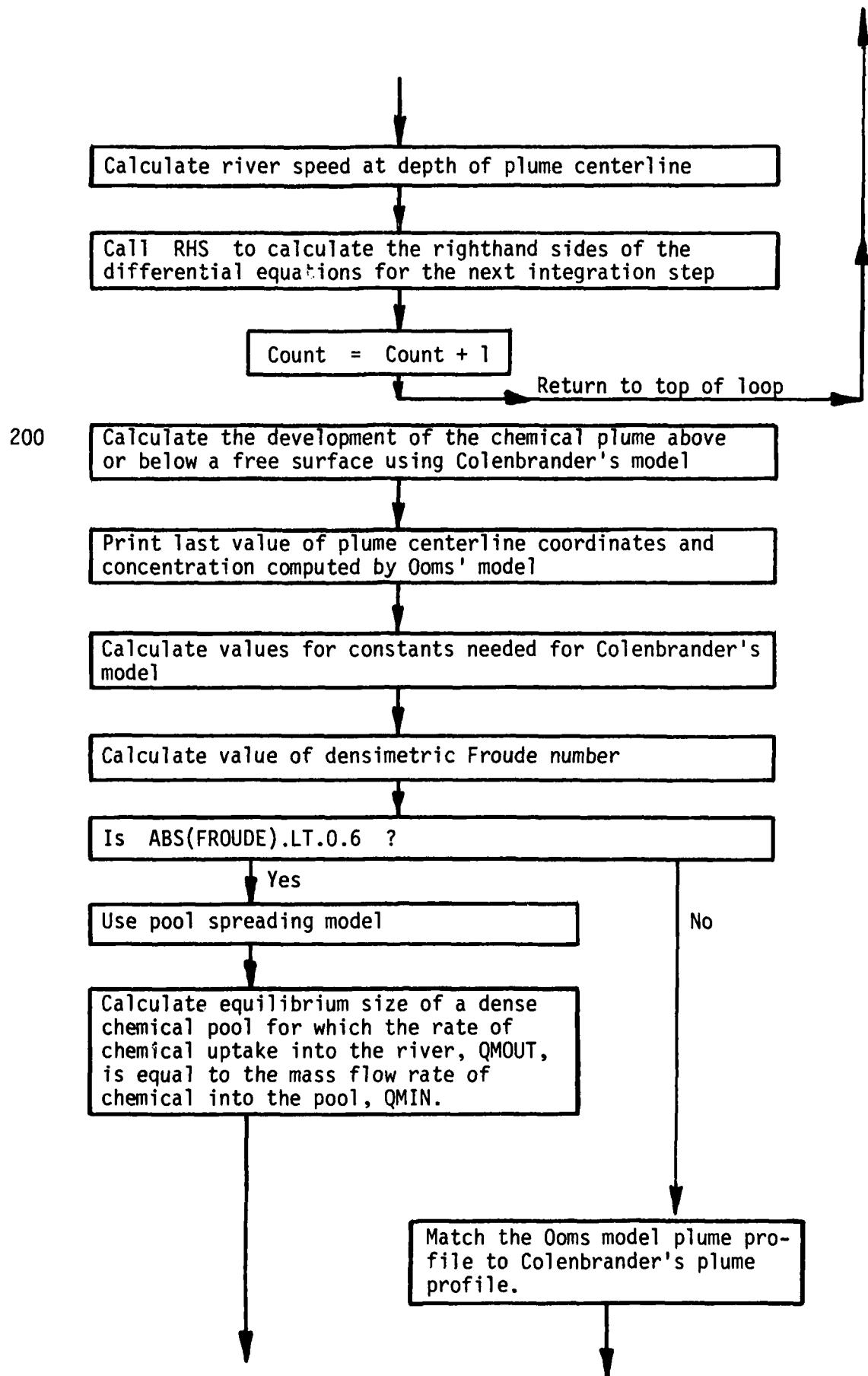
Yes

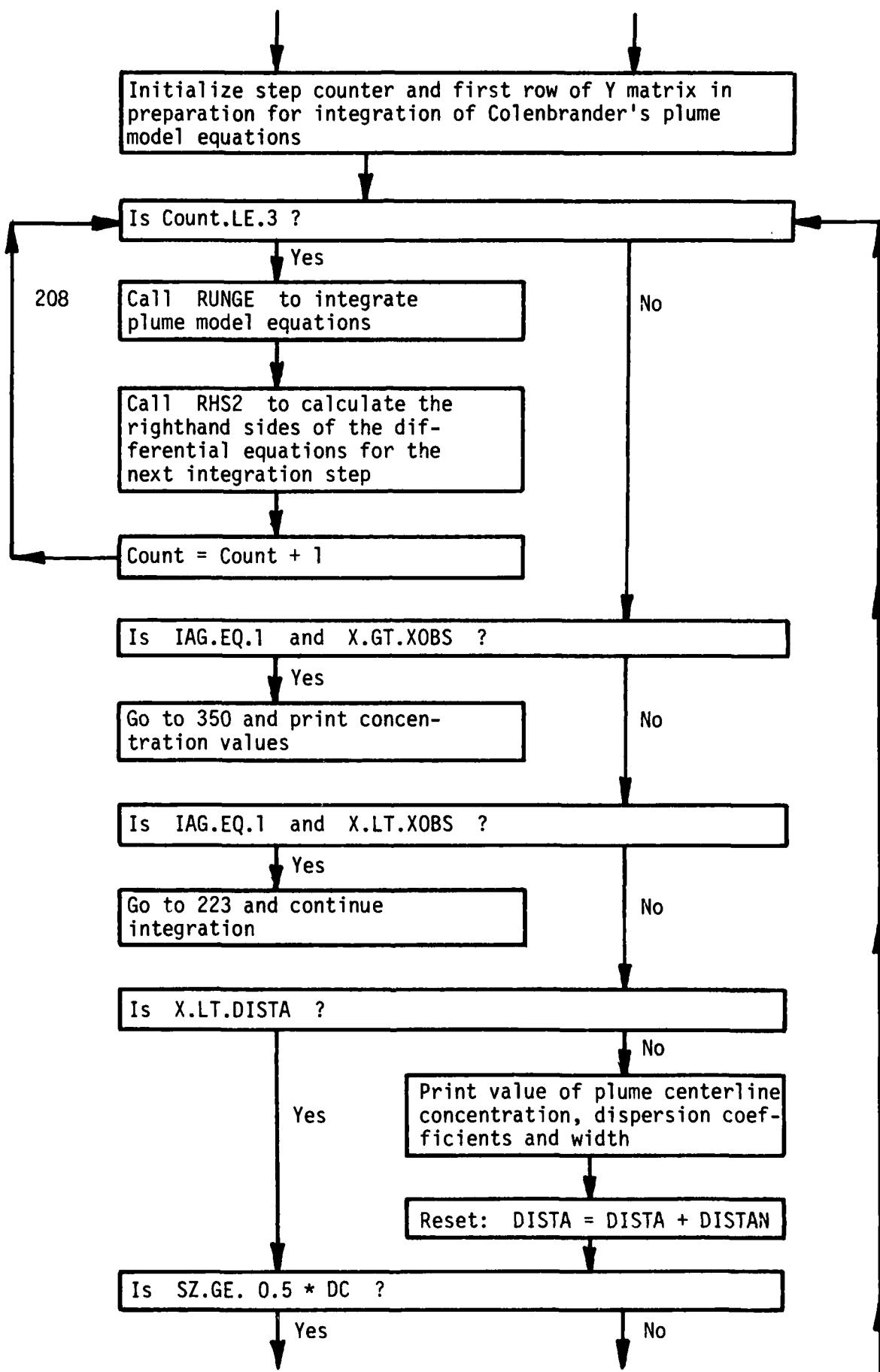
Go to 300

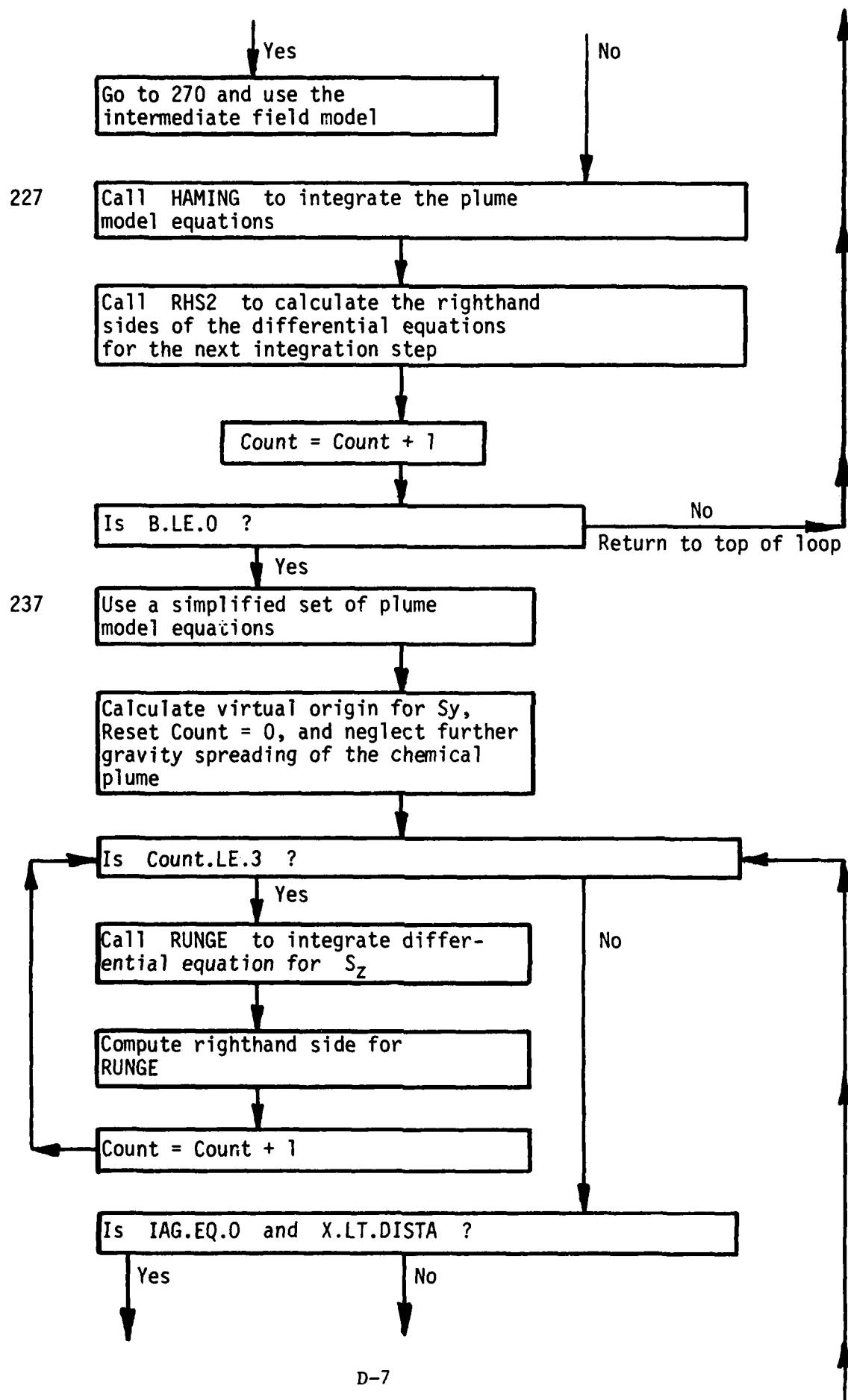
No

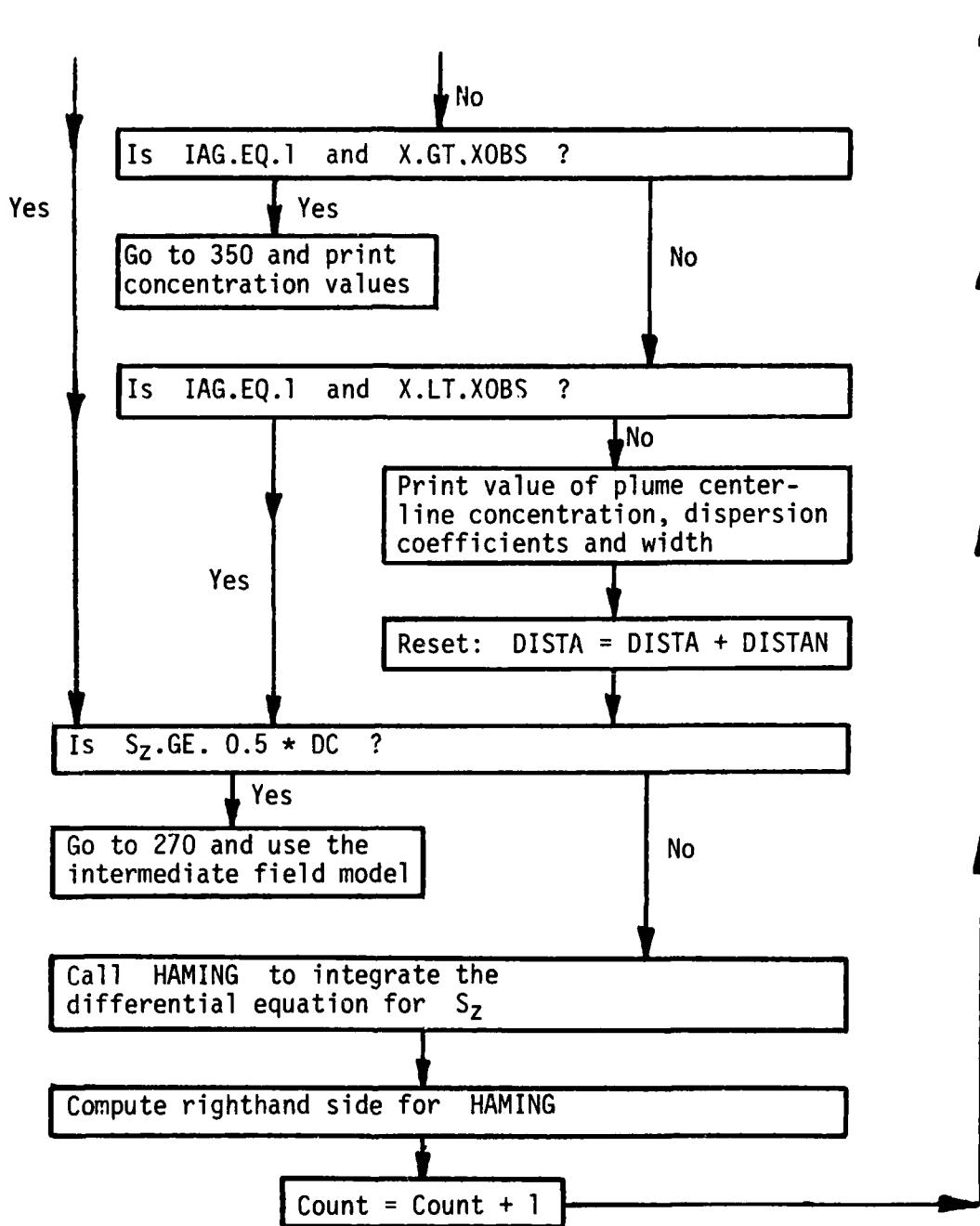
137

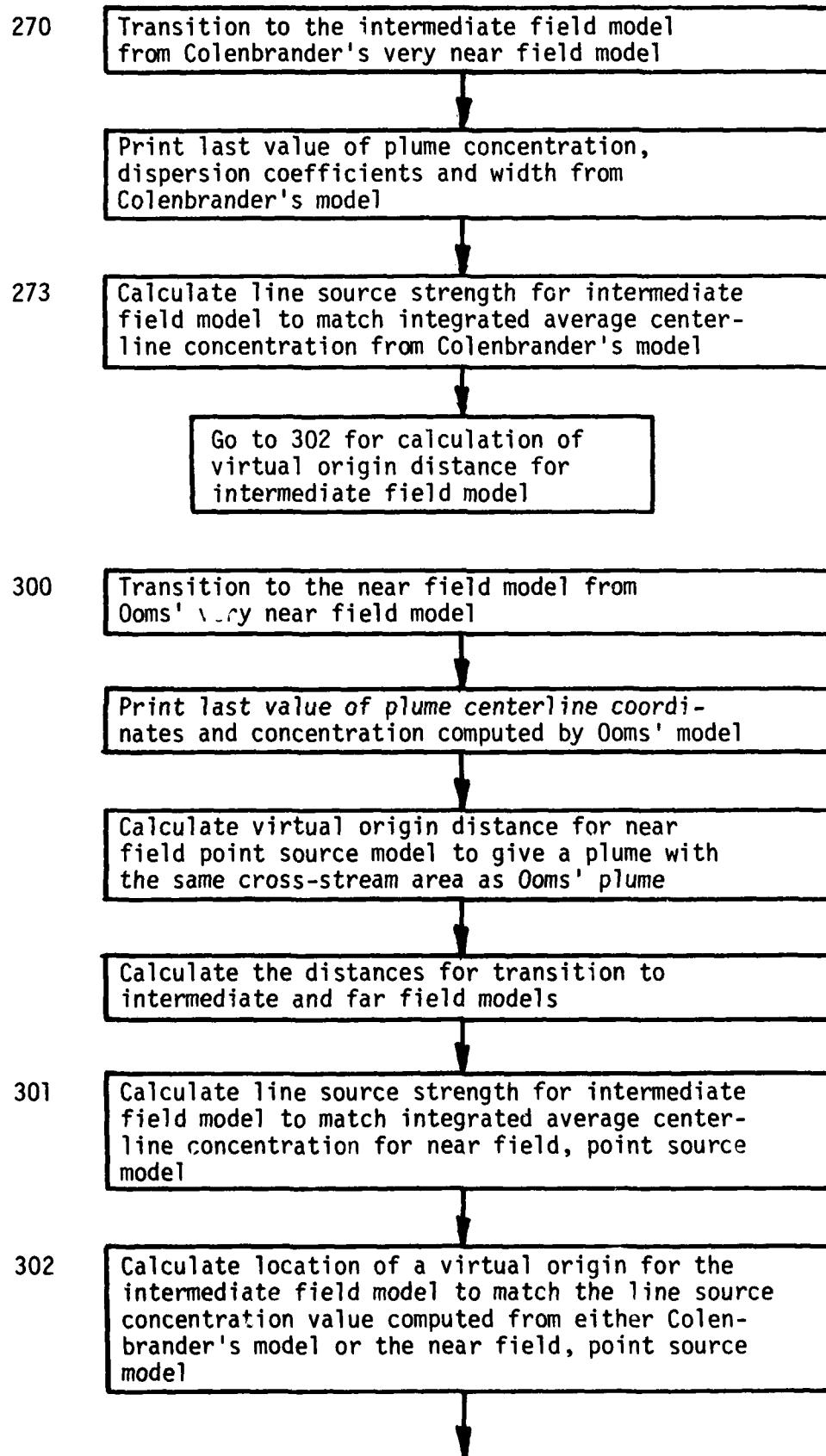
Call HAMING to integrate the plume model equations

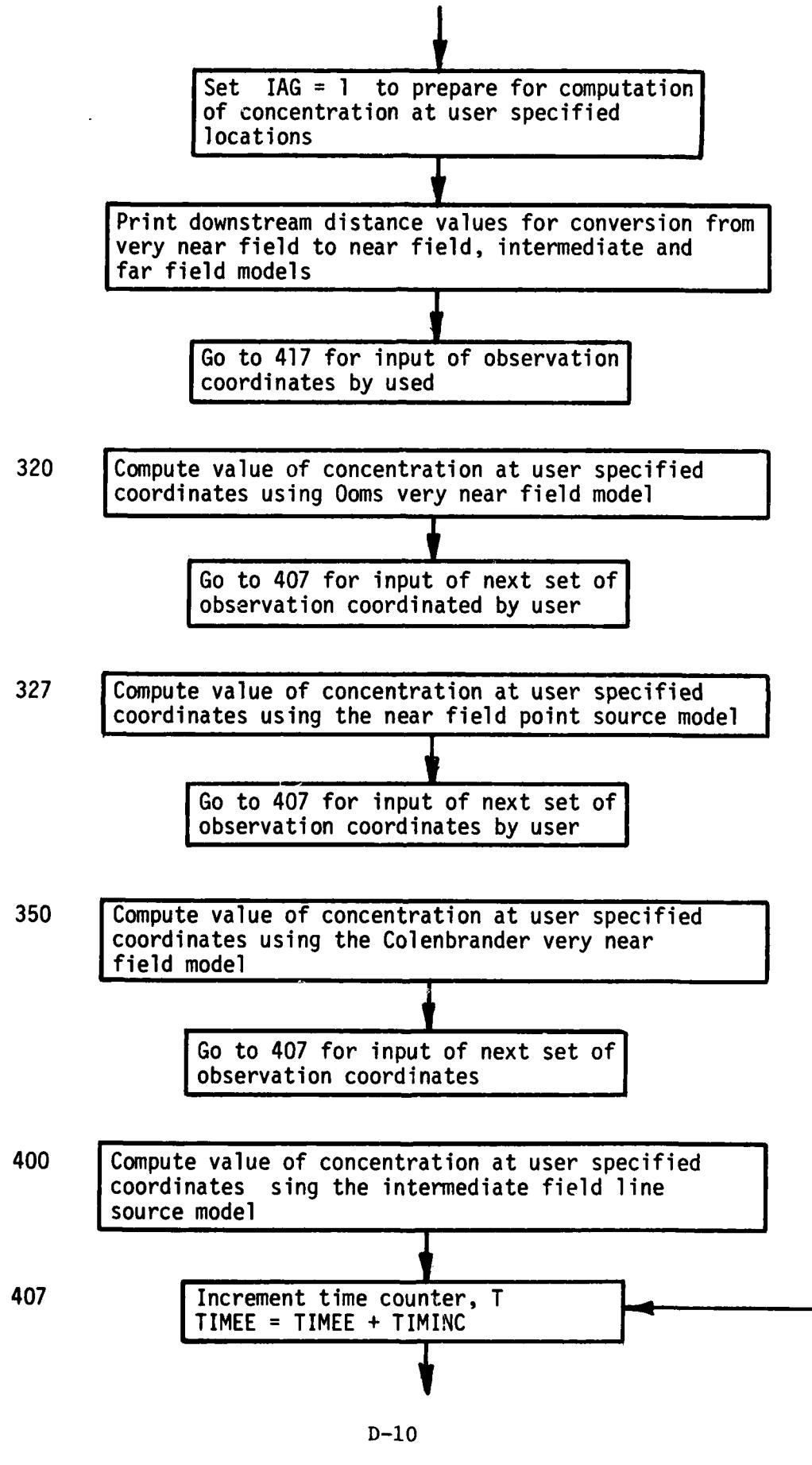


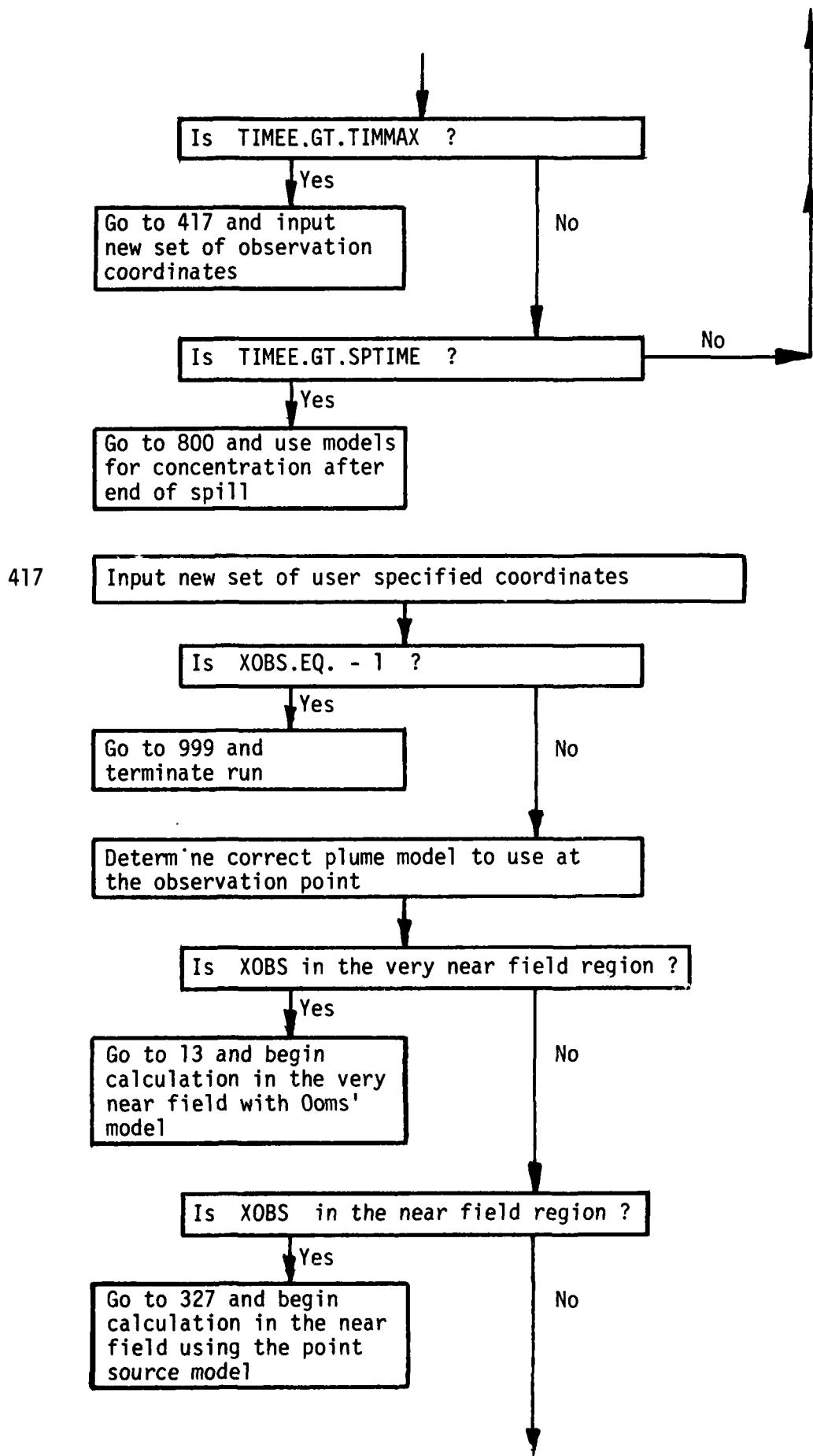












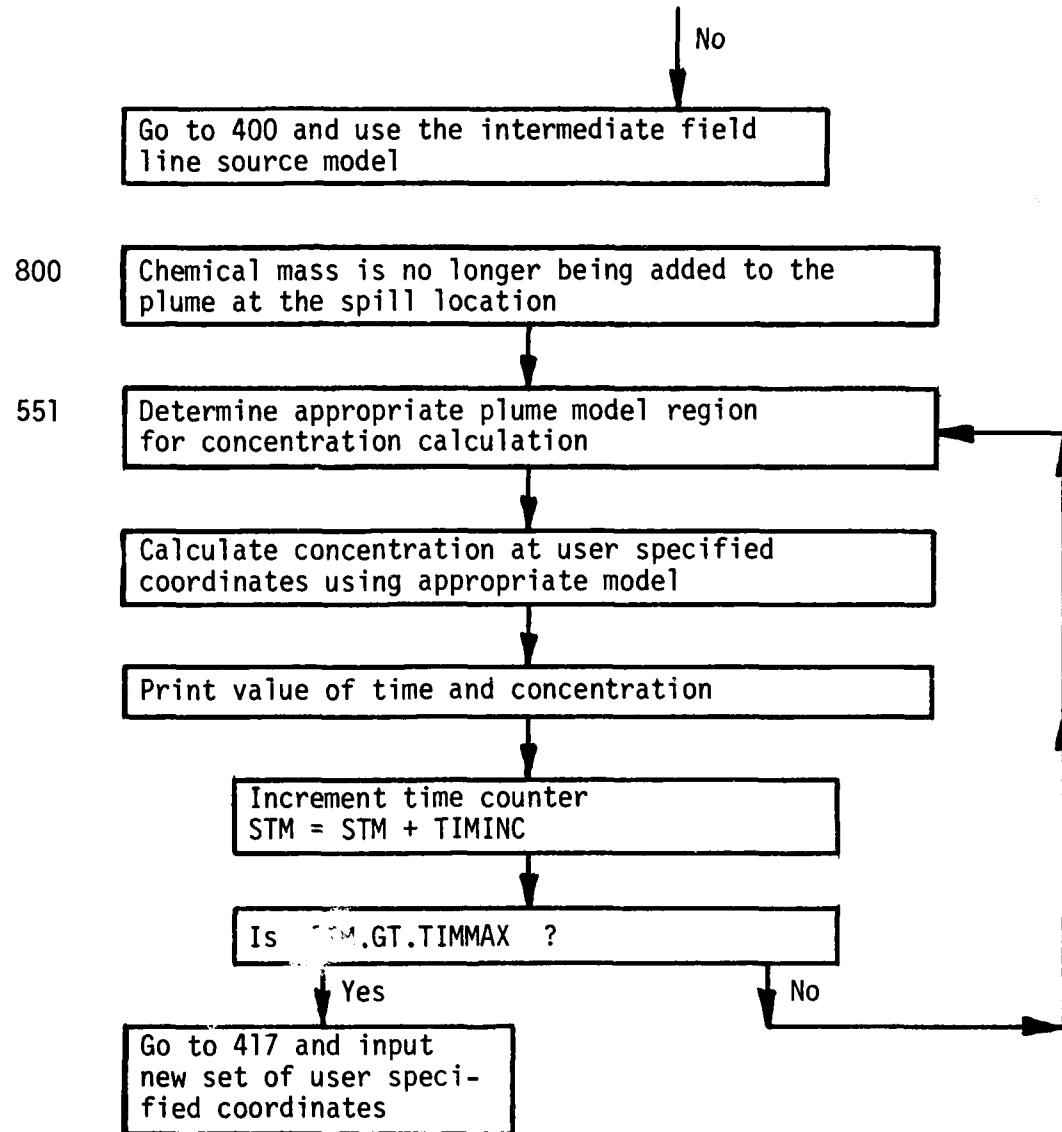
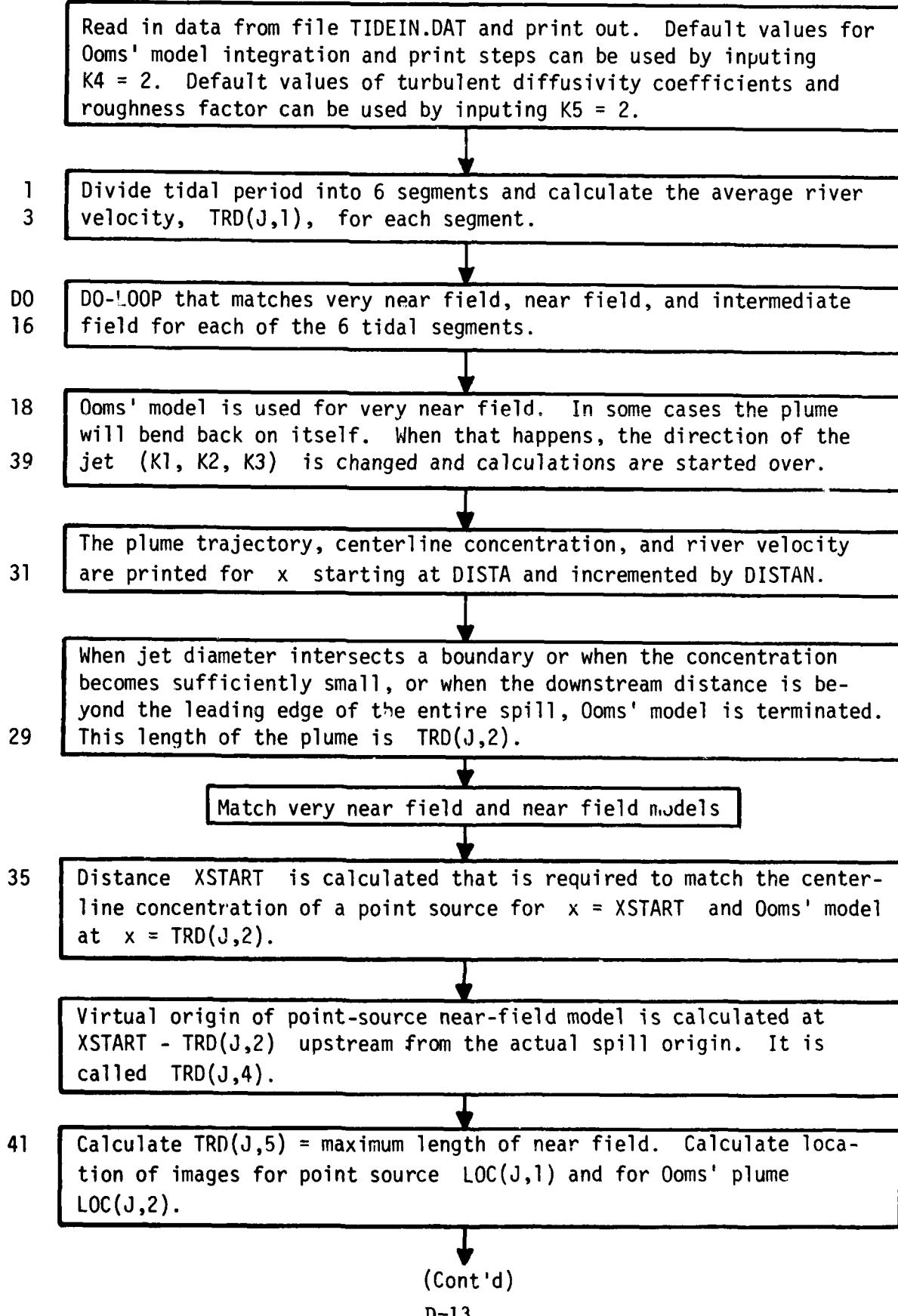


FIGURE D.3 FLOW CHART FOR PROGRAM "TIDAL"



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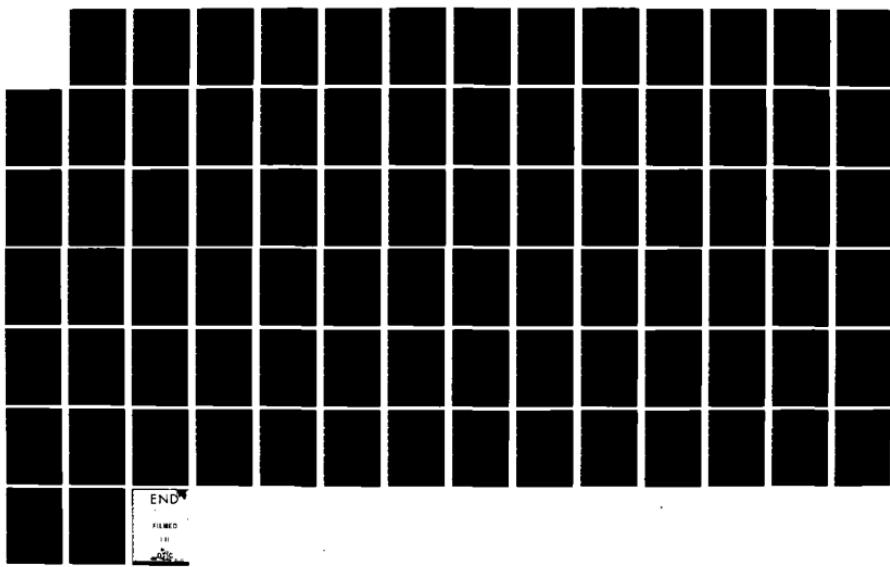
ANALYTICAL AND EXPERIMENTAL STUDY TO IMPROVE COMPUTER
MODELS FOR MIXING A. (U) SOUTHWEST RESEARCH INST SAN
ANTONIO TX F T DODGE ET AL. AUG 82 DOT-CG-920622-A

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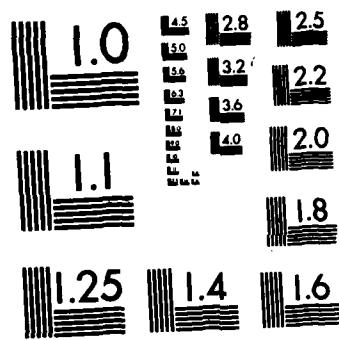
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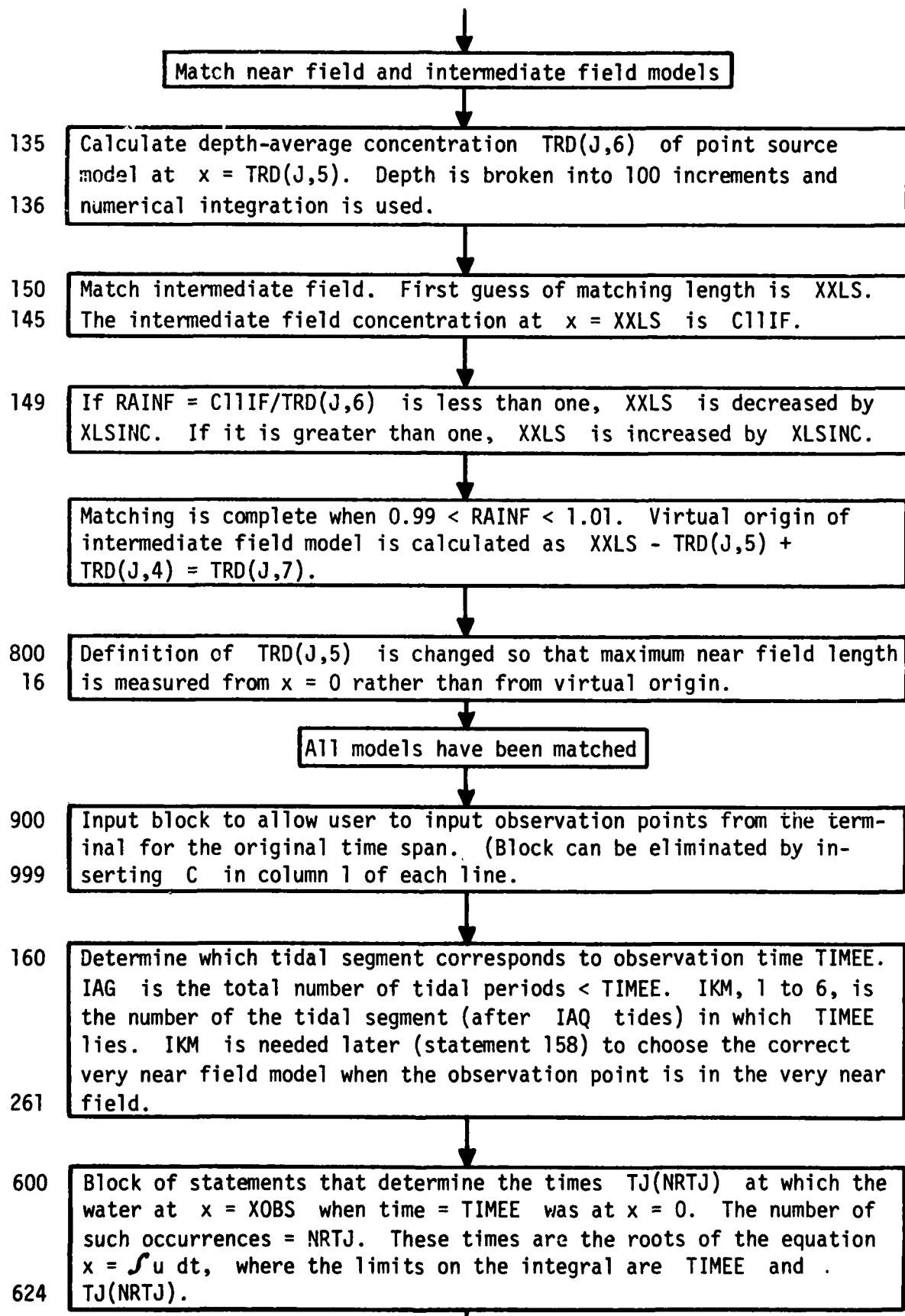
NL



END
FILED
100
AFC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A



340

Determine if the observation point is within the spill.

Is upstream edge $\leq X_{OBS} \leq$ downstream edge ?

No

Concentration = 0
To to 350

Yes

625

DO

620

Block of statements to determine in which tidal segments the roots
TJ(NRTJ) lie. IIIKM are the segment numbers.If the largest TJ(NRTJ) (i.e., most recent time, corresponding to
IEB = 1) is such that $|X_{OBS}| < TRD(IIIKM,2)$ = length of Ooms' model,
and the river velocity TRD(IIIKM,1) is the same direction as X_{OBS} ,
the most recent very near field model will contribute to the concen-
tration.is $\frac{TRD(IIIKM,1)}{X_{OBS}} > 0$ and $\frac{TRD(IIIKM,2)}{X_{OBS}} > 1$?

Yes

Set IVNF = 1
Go to 620

No

Is $TRD(IIIKM,2) > 1$?
(To check if river is in wrong direction.
If so, a near field model will be needed)

Yes

Set IIVNF = 1
To to 627

No

Is $\frac{TRD(IIIKM,5)}{X_{OBS}} > 1$?

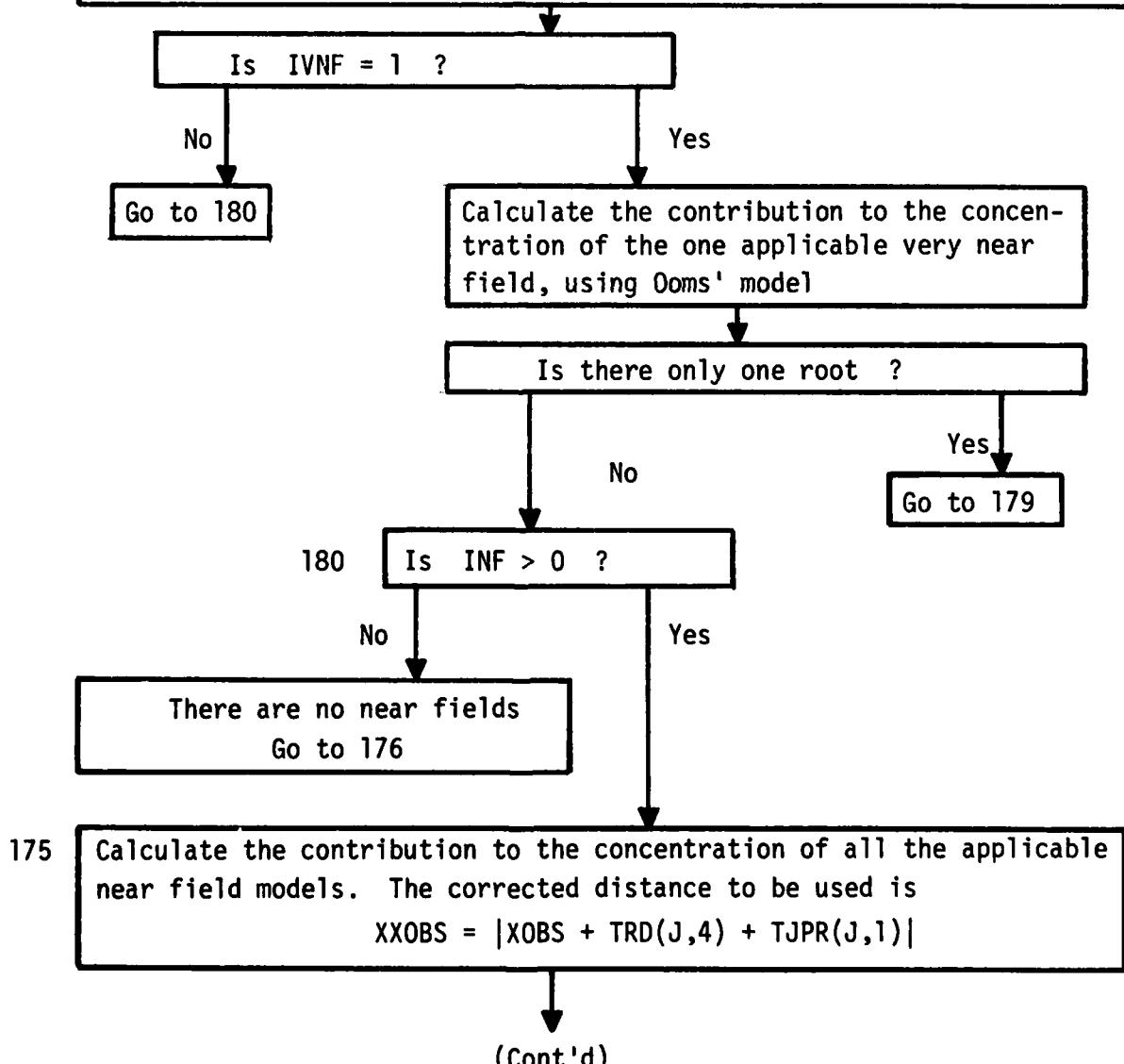
Yes

Go to 627

No

Go to 620

627 Block of statements that calculates the total absolute distance
 YY that the water travels in the period TIMEE - TJ(NRTJ).
 634 If IIVNF = 1 the extra distance (due to river direction reversals)
 that must be added to X0BS + TRD(J,4) (the distance from the
 virtual origin) is YY - TRD(J,2) = TJPR(IYZ,1). The number of
 applicable near fields, INF, is increased by one.
 631 If IIVNF = 0 (X0BS > very near field length), the extra distance
 that must be added is YY - TRD(J,5) = TJPR(IYZ,1). If this is
 < 0, the number of applicable near field models is increased by one,
 and no extra length must be added. If this is > 0, the root
 corresponds to an intermediate field, and TJPR(IYZ,1) must be
 added to the virtual origin of the intermediate field.



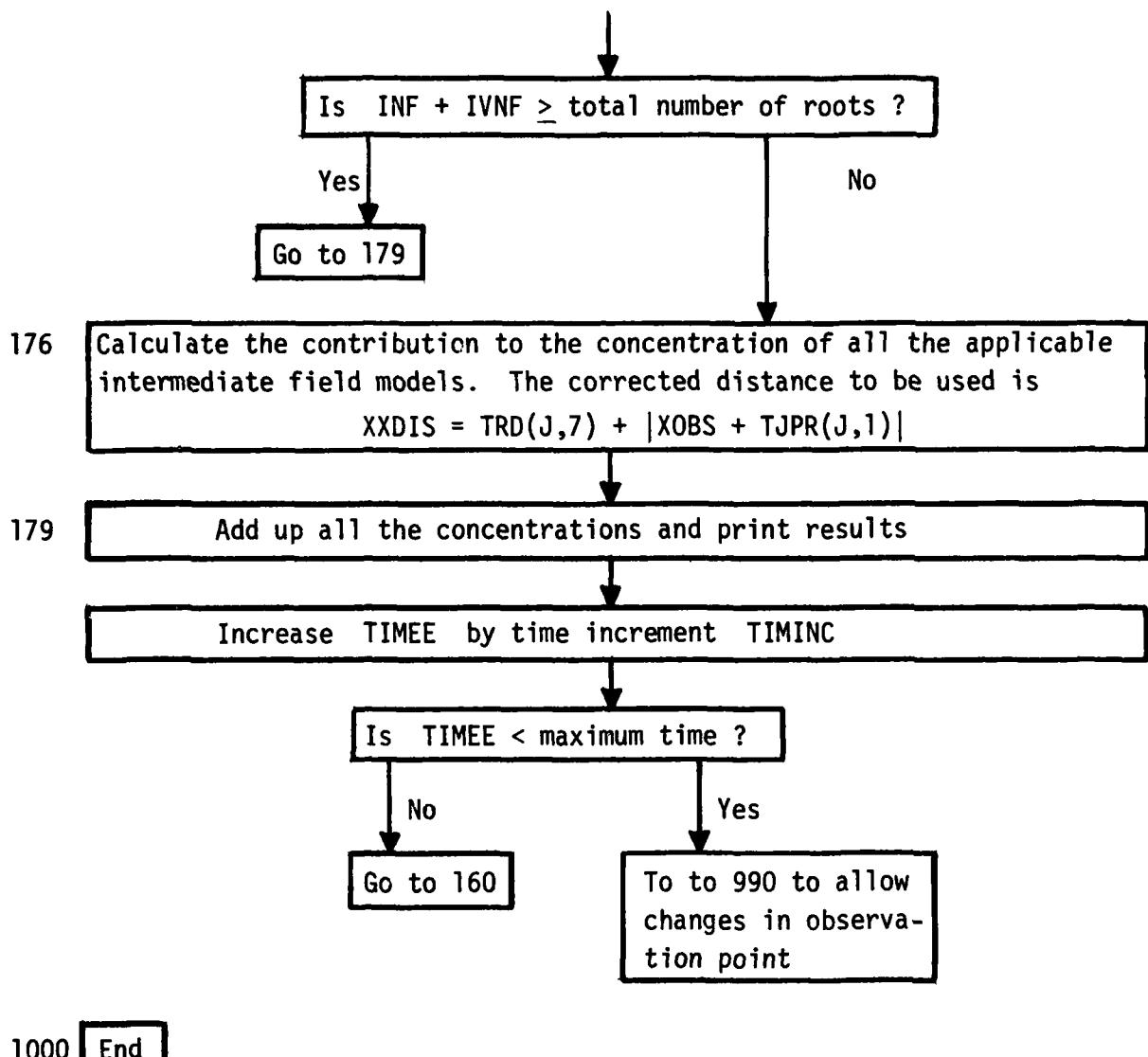
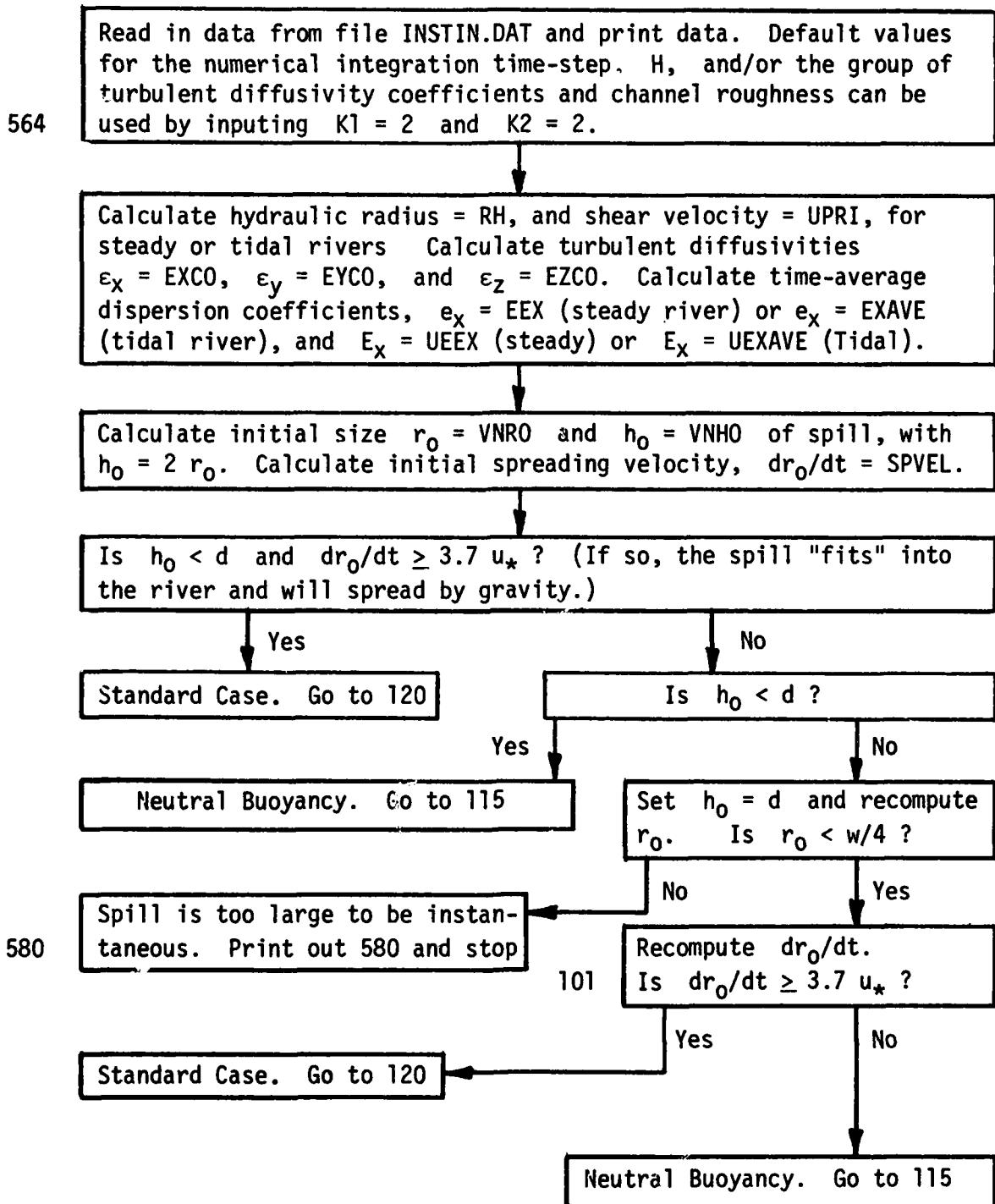
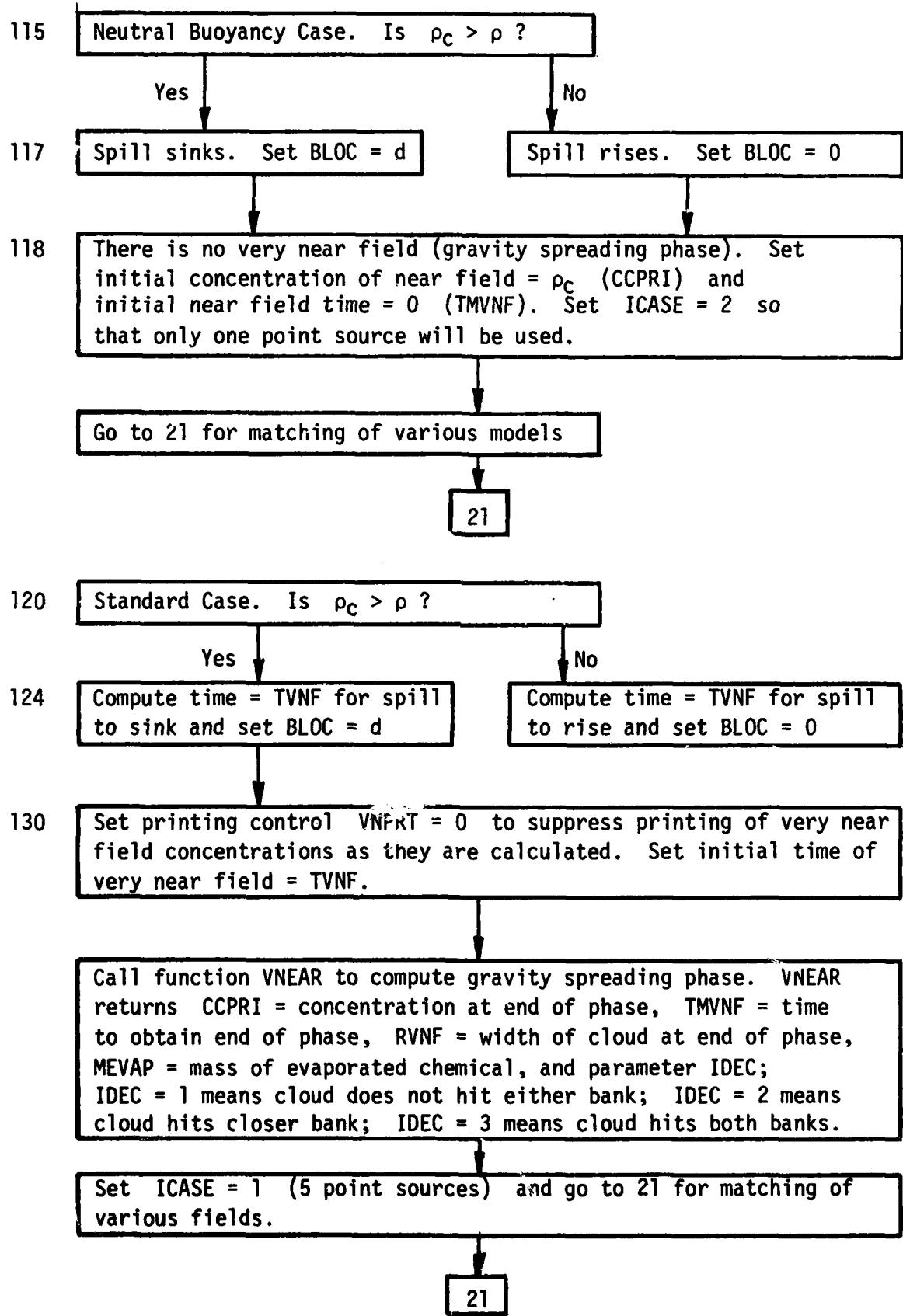
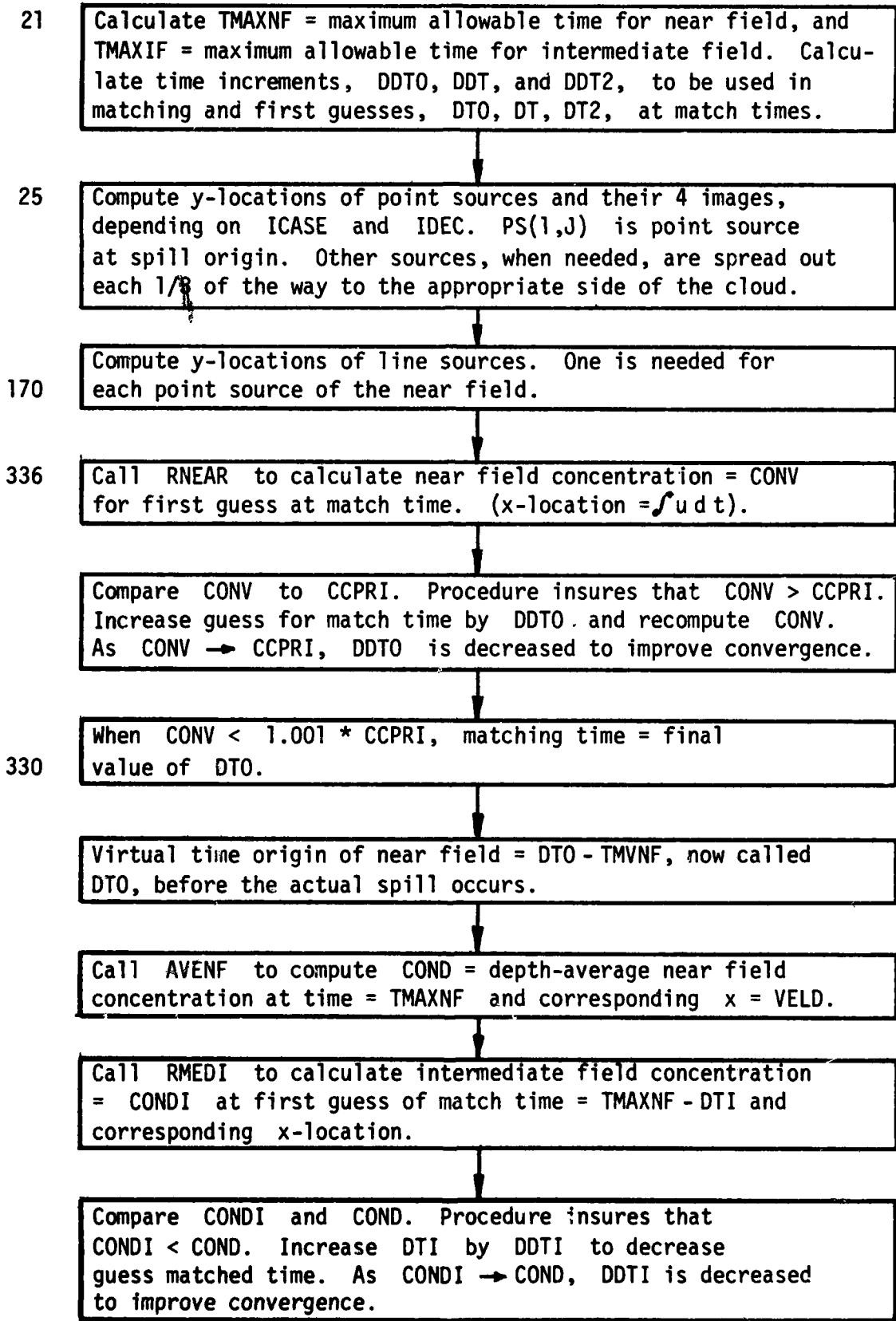


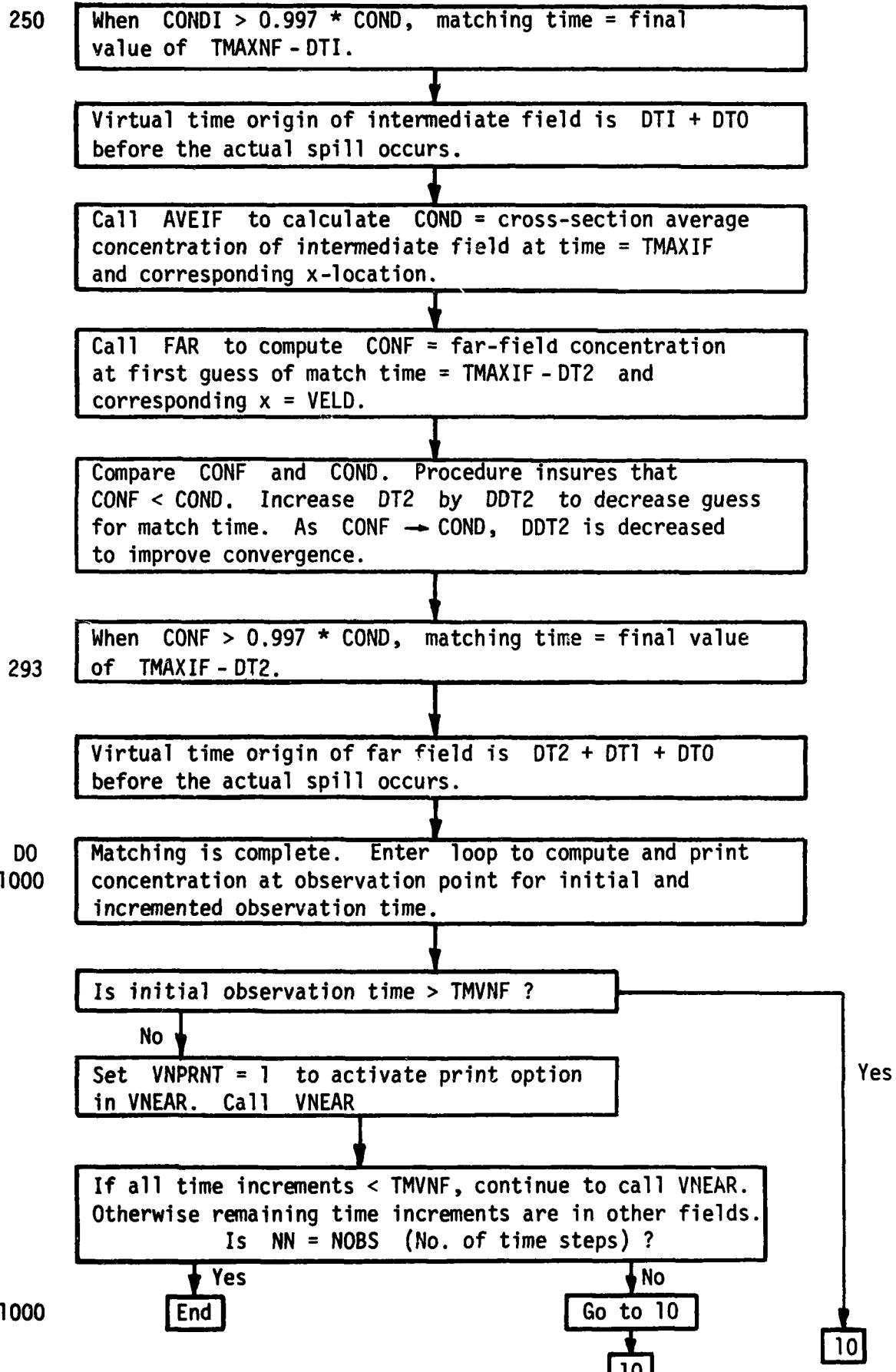
FIGURE D.4 FLOW CHART FOR PROGRAM "INSTANT"

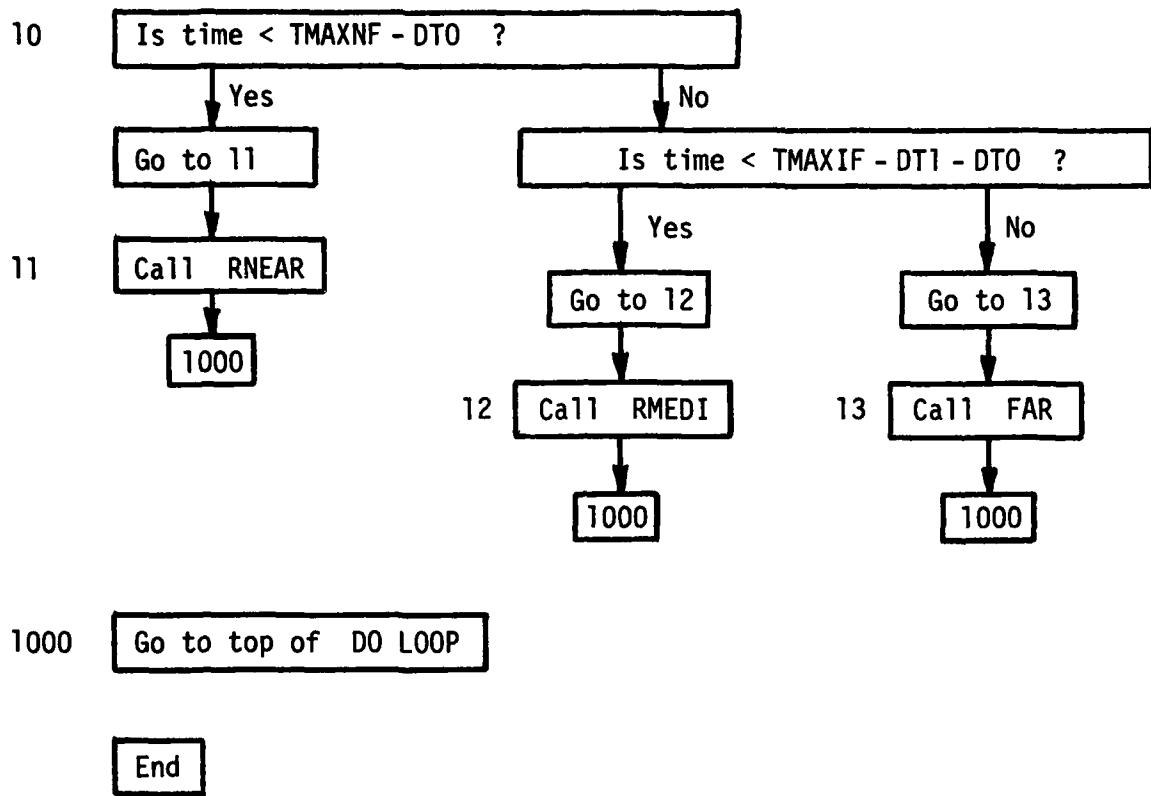






Cont'd.





Function RNEAR

Calculates concentration for a set of point sources, each having 4 images, at a given time, cross-stream location, downstream location, and depth. If the spill is neutrally buoyant only one point source is used, otherwise 5 are used. If spill is positively buoyant, spilled mass is reduced by evaporated mass.

Function RMEDI

Calculates concentration for a given set of vertical line sources, at a given time, cross-stream and downstream location. If the spill is neutrally buoyant, one line source is used, otherwise 5 are used. If spill is positively buoyant, spilled mass is reduced by evaporated mass.

Function FAR

Calculates concentration at a given time and downstream location when chemical is distributed uniformly over cross-section.

Function AVENF

Calculates average value of RNEAR over the river depth for a given time, cross-stream and downstream location.

Function AVEIF

Calculates average value of RMEDI for a given time and downstream location.

Function VELOC

Calculates value of \int_0^t (river speed * dt

Function ERRF

Calculated value of error function.

Function FACT

Calculates time-varying part of dispersion coefficient
for intermediate and far fields in a tidal river.

FIGURE D.5 FLOW CHART FOR PROGRAM "OOMS"

The function of this program is to provide four subroutines needed to calculate the mixing and dilution of bent-over plumes in a turbulent flowing stream by Ooms' method. The subroutines are HAMING, RUNGE, SIMUL and RHS.

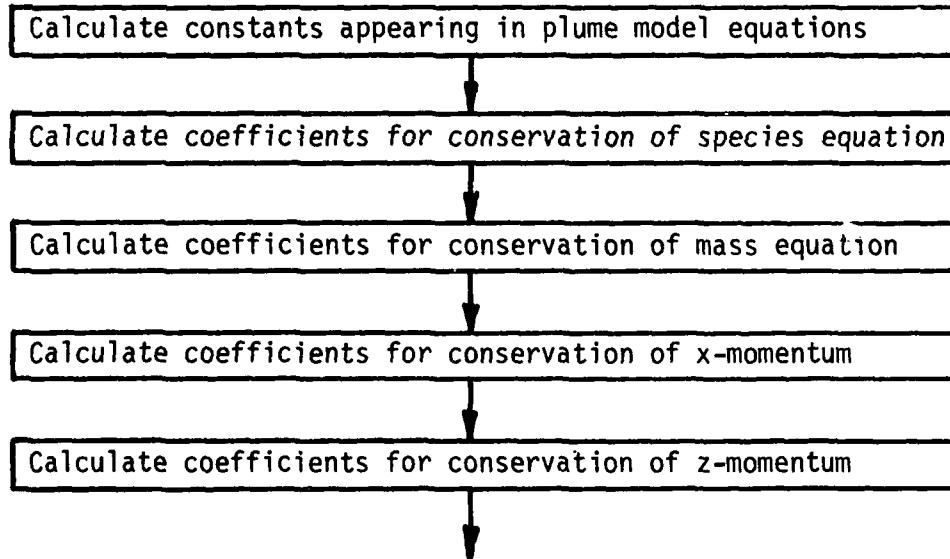
Subroutine RHS

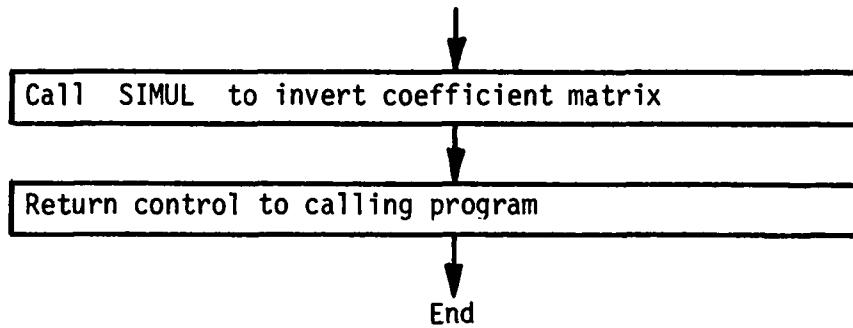
This subroutine computes values for the coefficients in the four simultaneous ordinary differential equations solved by Ooms method. The equations are of the form

$$A_{i1} \frac{dc_*}{ds} + A_{i2} \frac{db}{ds} + A_{i3} \frac{du_*}{ds} + A_{i4} \frac{d\theta}{ds} = A_{i5}$$

where $i = 1$, conservation of chemical species
 $i = 2$, conservation of mass
 $i = 3$, conservation of momentum in the x , downstream direction
 $i = 4$, conservation of momentum in the z , vertical direction
 c_* = plume centerline concentration
 b = plume characteristic radius
 u_* = plume velocity deficit
 θ = plume angle with respect to horizontal axis
 s = integration path along plume centerline axis

The sequence of operations is





Real Function SIMUL

This program is a general subroutine for solving matrix equations. It is called by subroutine RHS and is used to solve the matrix equation for the derivatives of plume concentration, $\frac{dc^*}{ds}$, etc. The function specification is

Real Function SIMUL (N,A,X,EPS,INDIC,NRC)

Function SIMUL is taken from "Applied Numerical Methods" by B. Carnahan, H. A. Luther, and J. O. Wilkes, published by J. Wiley and Sons, Inc., 1969, Pages 290 to 291.

Subroutine RHS sets N = 4, INDIC = 1, and NRC = 5 in the function call statement. The value of EPS is set in Program STEADY. The reader is referred to the text by Carnahan, et al. for a complete description of this function subroutine. The following paragraph is taken from the comment statements in the program listing.

When INDIC is negative, SIMUL computes the inverse of the N by N matrix A in place. When INDIC is zero, SIMUL computes the N solutions X(1)...X(N) corresponding to the set of linear equations with augmented matrix of coefficients in the N by N+1 array A and in addition computes the inverse of the coefficient matrix in place as above. If INDIC is positive, the set of linear equations is solved but the inverse is not computed in place. The Gauss-Jordan complete elimination method is employed with the maximum pivot strategy. Row and column subscripts of successive pivot elements are saved in order in the IROW and JCOL arrays, respectively. K is the pivot counter, PIVOT the algebraic value of the pivot element, MAX the number of columns in A, and DETER the determinant of the coefficient matrix. The solutions are computed in the (N+1) th column of A and then unscrambled and put in proper order in X(1)...X(N) using the pivot subscript

information available in the IROW and JCOL arrays. The sign of the determinant is adjusted, if necessary, by determining if an odd or even number of pairwise interchanges is required to put the element of the JORD array in ascending sequence where $JORD(IROW(I)) = JCOL(I)$. If the inverse is required, it is unscrambled in place using $Y(1) \dots Y(N)$ as temporary storage. The value of the determinant is returned as the value of the function. Should the potential pivot of largest magnitude be smaller in magnitude than EPS, the matrix is considered to be singular and a true zero is returned as the value of the function.

Integer Function RUNGE

This program is a general subroutine for solving a set of first order ordinary differential equations. It is called by program STEADY, and is used to start the solution of the set of plume development equations. After three forward steps are completed, subroutine HAMING is used instead of RUNGE to continue the numerical integration. The function specification is

Integer Function RUNGE (N,Y,F,X,H)

Function RUNGE is taken from "Applied Numerical Methods" by B. Carnahan, H. A. Luther, and J. O. Wilkes, published by J. Wiley and Sons, Inc., 1969, Pages 374 to 375.

The value of N is set in the function call statement. The value of H, the integration step size is either input or assigned a default value in STEADY. The reader is referred to the text by Carnahan, et al. for a complete description of this function subroutine. The following paragraph is taken from the comment statement in the program listing.

The function RUNGE employs the fourth-order Runge-Kutta method with Kutta's coefficients to integrate a system of N simultaneous first order ordinary differential equations $F(J) = DY(J)/DX$, ($J=1,2,\dots,N$), across one step of length H in the independent variable X, subject to initial conditions $Y(J)$, ($J=1,2,\dots,N$). Each $F(J)$, the derivative of $Y(J)$, must be computed four times per integration step by the calling program. The function must be called five times per step (Pass (1)...Pass(5)) so that the independent variable value (X) and the solution values ($Y(1) \dots Y(N)$) can be updated using the Runge-Kutta algorithm. M is the pass counter. RUNGE returns as its value 1 to signal that all derivatives (the $F(J)$) be evaluated or 0 to signal that the integration process for the current step is finished. SAVEY(J) is used to save the initial value of $Y(J)$ and PHI(J) is the increment function for the $J(TH)$ equation. As written, N may be no larger than 50.

Integer Function HAMING

This program is a general subroutine for solving a set of first order ordinary differential equations. It is called by subroutine STEADY, and is used to continue the solution of the set of plume development equations after RUNGE has provided the set of initial values. The function specification is

Integer Function HAMING (N,Y,F,X,H,TE)

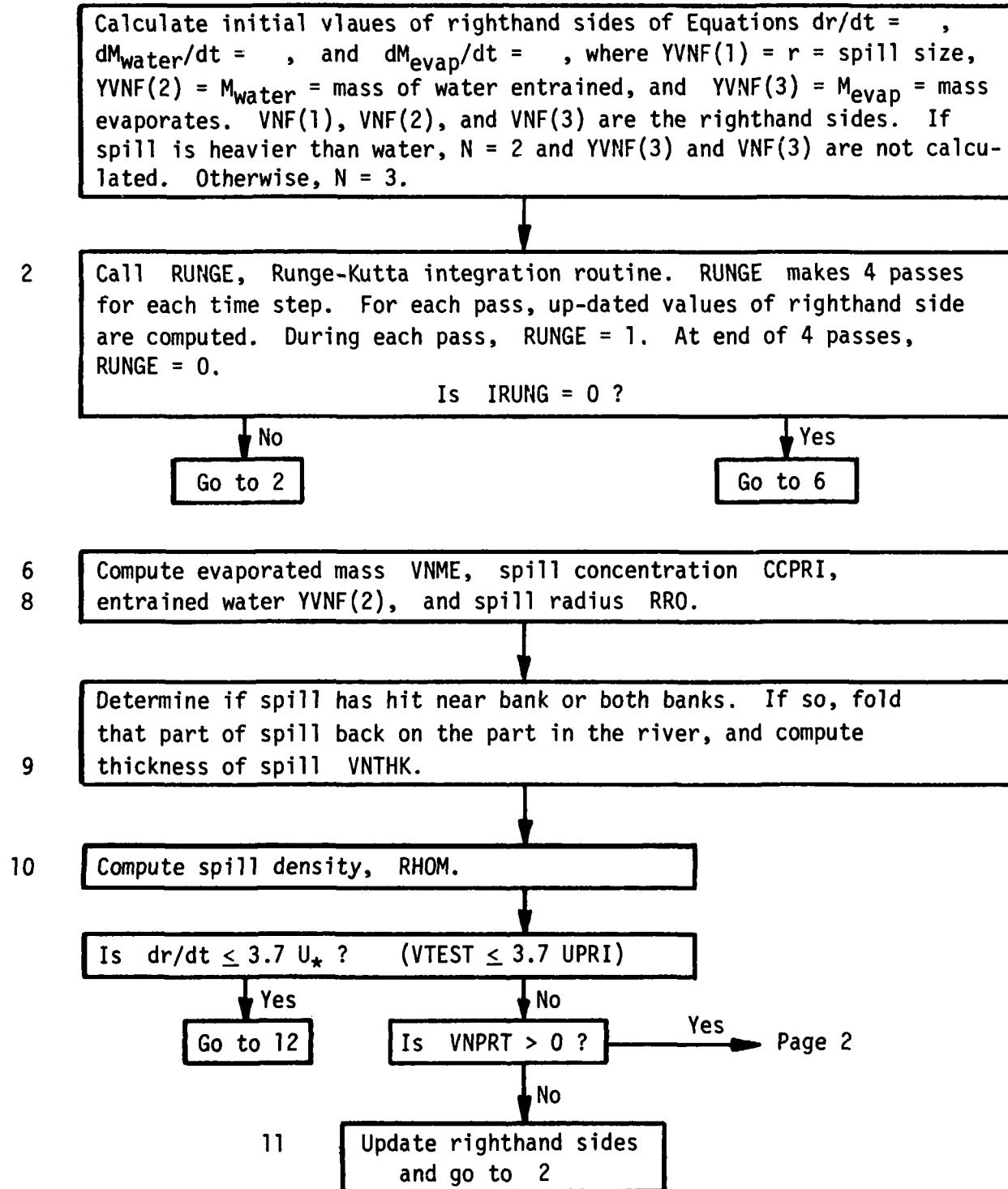
Function HAMING is taken from "Applied Numerical Methods" by B. Carnahan, H. A. Luther, and J. O. Wilkes, published by J. Wiley and Sons, Inc., 1969, Pages 401 to 402.

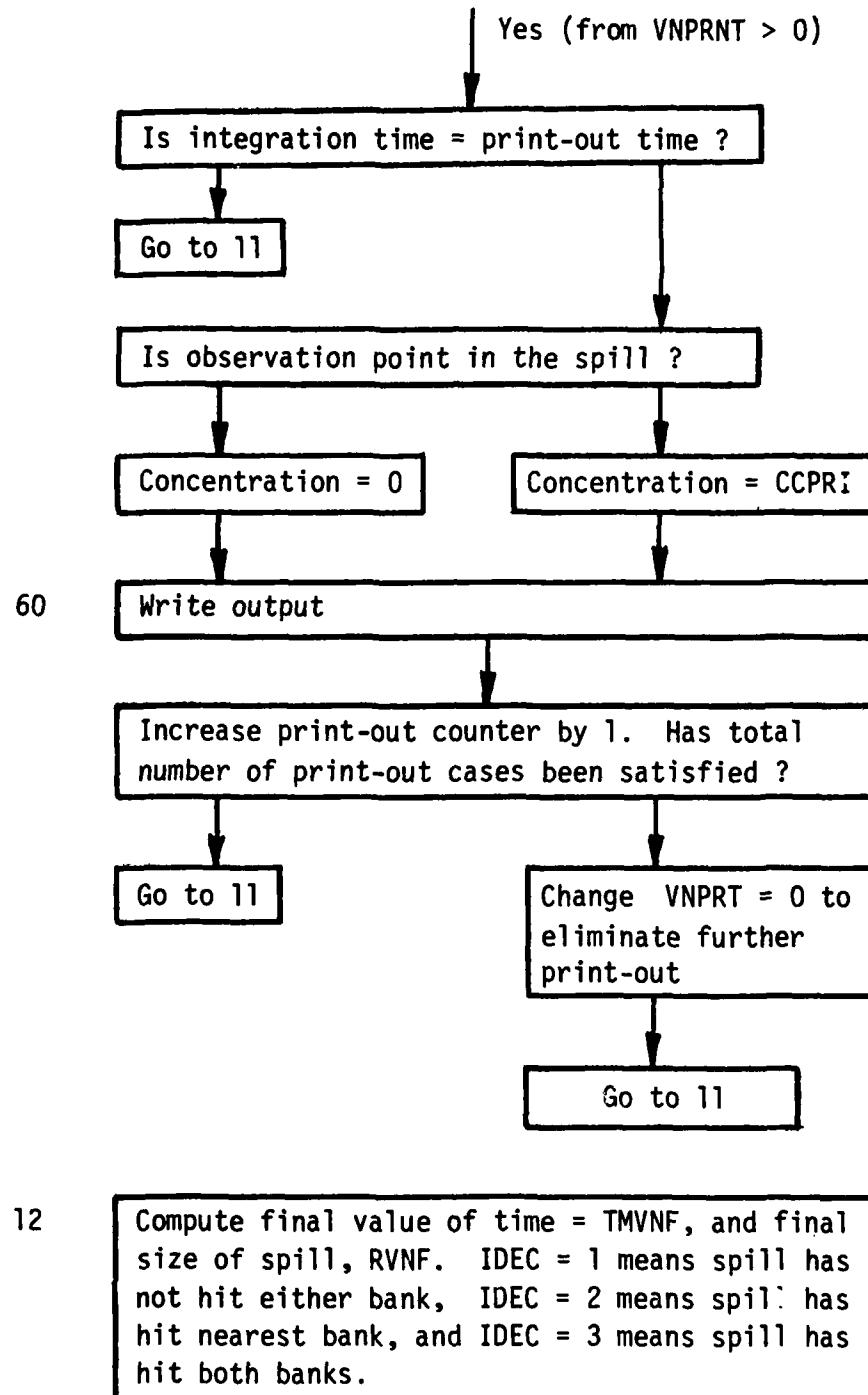
The value of N is set in the function call statement. The value of H, the integration step size is either input or assigned a default value in program STEADY. The reader is referred to the text by Carnahan, et al. for a complete description of this function subroutine. The following paragraph is repeated from the program listing.

HAMING implements Hamming's predictor-corrector algorithm to solve N simultaneous first-order ordinary differential equations. X is the independent variable, and H is the integration stepsize. The routine must be called twice for integration across each step. On the first call, it is assumed that the solution values and derivative values for the N equations are stored in the first N columns of the first four rows of the Y matrix and the first three rows of the F matrix, respectively. The routine computes the N predicted solutions YPRED(J), increments X by H and pushes all values in the Y and F matrices down one row. The predicted solutions YPRED(J) are modified, using the truncation error estimates TE(J) from the previous step, and saved in the first row of the Y matrix. HAMING returns to the calling program with the value 1 to indicate that all derivatives should be computed and stored in the first row of the F array before the second call is made on HAMING. On the second entry to the function (determined by the logical variable PRED), HAMING uses the Hamming corrector to compute new solution estimates, estimates the truncation errors TE(J) for the current step, improves the corrected solutions using the new truncation error estimates, saves the improved solutions in the first row of the Y matrix, and returns to the calling program with a value 2 to indicate completion of one full integration step.

FIGURE D.6 FLOW CHART FOR FUNCTION "VNEAR"

This function calculates concentration of a non-neutrally buoyant instantaneous spill undergoing gravity spreading. Used by INSTANT.





APPENDIX E

COMPUTER PROGRAM LISTINGS

```
DIAJET=XXXX. XXXX
K4=II
X=XXXXX. XXXX  H=XXX. XXXXXX
DISTA=XXXXXXX. XXXX  DISTAN=XXXXXXX. XXXX
ROA=XXXXX. XXX  DENS=XXXXX. XXX
TEST
AAAAAAA1AAA1AAA1AAAAAAA1AAAAAAA1
TESTNO=AAAAAAA
GINIT=8 . XXXXE+XX  SPTIME=XXXXXXXX. X  TIMINC= XXXXXXXX. X
TIMMAX=XXXXXXXX. X  TPER=XXXXXXXX. X
WC=XXXXX. XXX  DC=XXXXX. XXX
XOBS=XXXXXXXX. X  YOBS=XXXXXX. XXX  ZOBS=XXXXXX. XXX
ALOC=XXXXXX. XXX  BLOC=XXXXXX. XXX
K5=II
EYCOEF=XXXX. XXXXX  EZCOEF=XXXX. XXXXX  VNUM=XXXX. XXXXX
U1NF=XXXXXX. XX  U2NF=XXXXXX. XX  ALFANF=XXXXX. XXXX
K1=II  K2=II  K3 II
```

NOTE: II = Integer Type Input
XX.XX = Fixed Point Type Input
AAAA1 = ALPHA-NUMERIC Type Input

DUMMY INPUT FORM FOR PROGRAM "TIDAL"

```
K1=II
WC=XXXXXX. XXX  DC=XXXXXX. XXX
H=XXX. XXXXXX
ROA=XXXXXX. XXX  DENS=XXXXXX. XXX
AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1
TESTNO=AAAAAAA1
ALOC=XXXXXX. XXX  BLOC=XXXXXX XXX
K2=II
EYCOEF=XXXX. XXXXX  EZCOEF=XXXX. XXXXX  VNUM=XXXX. XXXXX
U1NF=XXXX. XXX  U2NF=XXXXXX. XX  ALFANF=XXXXX. XX  TPER=XXXXXXXX. XX
NOBS=III
AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1
XOB=XXXXXXXX. XXXX  YOB=XXXXXXXX. XXXX  ZOB=XXXXXXXX. XXXX
TLOW=XXXXXXXX. XX  TDELT=XXXXXXXX. XX  NSTEP=IIIIII
SMASS=XXXXXX. XXXX  HEVAP=XXXXXX. XXXX
```

NOTE: (1) II = Integer Type Input
XX.XX = Fixed Point Type Input
AAAA1 = ALPHA-NUMERIC Type Input
(2) ** = Blank Line; will not be
read as input

DUMMY INPUT FORM FOR PROGRAM "INSTANT"

```
X=XXXXXX. XXX H=XXXXXX. XXX DISTA=XXXXXX. XXX DISTAN=XXXXXX. XXX
RCA=XXXXXX. XXX DEN8=XXXXXX. XXX TO=XXX. X UR=XXXX. XXX
TESTNO=AAAAAAA1
AAAAAAA1AAAAAAA1AAAAAAA1AAAAAAA1
DIAJET=XXXXXX. X GINIT=5X. XXXXE+XX SPTIME=XXXXXXXX. X
TIMING=XXXXXXXX. X TIMMAX=XXXXXXXX. X
WC=XXXXXX. XXX DC=XXXXXX. XXX ALOC=XXXXXX. XXX BLOC=XXXXXX. XXX
KNF=XXXX. XXXXX KIF=XXXX. XXXXX KFF=XXXX. XXXXX
EYCOEF=XXXX. XXXXX EZCOEF=XXXX. XXXXX SLCNC=XX. XXX XLSINC=XXX. XXX
K1=II K2=II K3=II
```

NOTE: II = Integer Type Input
XX.XX = Fixed Point Type Input
AAAA1 = ALPHA-NUMERIC Type Input

DUMMY INPUT FORM FOR PROGRAM "STEADY"

```

C *****PROGRAM SPILL *****
C
C THIS MAIN PROGRAM CALLS THE APPROPRIATE DILUTION MODEL
C (STEADY, TIDAL, INSTANT) FOR COMPUTING THE CHEMICAL
C CONCENTRATION SPILLED INTO A WATERWAY. IT ALSO
C CONTAINS SUBROUTINE "JET" WHICH ADJUSTS THE VELOCITY
C PROFILE AND DIAMETER OF A CONTINUOUS DISCHARGE FROM
C A CIRCULAR PUNCTURE (CALLED BY "STEADY" AND "TIDAL")
C AND SUBROUTINE "COEF" WHICH CALCULATES THE TIME-
C AVERAGE DIFFUSION AND DISPERSION COEFFICIENTS
C (CALLED BY "STEADY" AND "TIDAL")
C
C
C OUTPUT FILE NAMES: SPILLOUT.DAT
C
C OPEN(UNIT=3, NAME='SYO: SPILLOUT.DAT')
C
C OUTPUT FILE SPILLOUT.DAT IS USED BY STEADY, TIDAL,
C AND INSTANT.
C
C DETERMINE IF THE STEADY OR TIDAL MODEL SHOULD BE USED.
C
C TYPE*, 'SELECT THE MODEL TO BE USED:
C TYPE*, ' 1. STEADY'
C TYPE*, ' 2. TIDAL '
C TYPE*, ' 3. INSTAN'
C TYPE*, 'ENTER THE NUMBER CORRESPONDING TO THE DESIRED MODEL
C ACCEPT*, NMLKJI
C IF (NMLKJI, EQ. 1) CALL STEADY
C IF (NMLKJI, EQ. 2) CALL TIDAL
C IF (NMLKJI, EQ. 3) CALL INSTAN
C CALL EXIT
C END
C SUBROUTINE JET (YR, UR, QINIT, DIAJET, ROA, K1, K2, K3, ALOC, BLOC, DC)
C REAL JAY
C DIMENSION YR(6), XOD(10), ZOD(10), PATHL(10)
C UV=1. 2732*QINIT/((DIAJET/100.0)**2.0)
C JAY=(YR(1)/ROA)*(UV/UR)**2.0
C AV=EXP(0. 405465+0. 207519*ALOC(JAY))
C ROW=0. 871667+0. 1775*(UV/UR)
C XOD(0)=0. 0
C ZOD(0)=0. 0
C PATHL(0)=0. 0
C I=0
C 40 I=I+1
C XOD(I)=XOD(I-1)+0. 10
C ZOD(I)=AV*XOD(I)**0. 4
C PATHL(I)=PATHL(I-1)+SQRT((XOD(I)-XOD(I-1))**2. 0+(ZOD(I)-ZOD(I-1))
C 1**2. 0)
C IF (PATHL(I), LT. ROW) GO TO 40
C FXOD=XOD(I-1)+(XOD(I)-XOD(I-1))*((ROW-PATHL(I-1))/(PATHL(I)-
C 1*PATHL(I-1)))
C YR(2)=(DIAJET/100.0)*SQRT(1.0/(4.0*(0.556796+0.486344*UR*1
C COS(YR(4))/UV)))
C IF (K3, EQ. 1. OR. K3, EQ. -1) GO TO 47
C YR(5)=FXOD*DIAJET/100.0
C IF (K1, NE. -1) GO TO 41
C YR(5)=-YR(5)
C 41 IF (K2, EQ. 1) GO TO 42
C IF (K2, EQ. -1) GO TO 43
C YR(6)=BLOC
C GO TO 44

```

```

42 YR(6)=-AV*((ABS(FXOD)**0.4)*(DIAJET/100.0)+BLOC
    GO TO 44
43 YR(6)=(AV*((ABS(FXOD)**0.4)*(DIAJET/100.0)+BLOC
44 CONTINUE
    IF (YR(6).LT.0.0) GO TO 45
    IF (YR(6).GT.DC) GO TO 45
    IF (K1.EQ.1.OR.K1.EQ.-1.0) YR(4)=0.0
    IF (K2.EQ.1) YR(4)=ATAN(AV*0.4*(ABS(FXOD)**(-0.6)))
    IF (K2.EQ.-1) YR(4)=-ATAN(AV*0.4*(ABS(FXOD)**(-0.6)))
    YR(3)=UV-UR+COS(YR(4))
    GO TO 46
45 YR(3)=UV-UR
    YR(4)=0.0
    YR(5)=0.0
    YR(6)=BLOC
    GO TO 46
47 YR(5)=0.0
    YR(6)=BLOC
    ALDC=ALOC+FXOD*DIAJET/100.0
    IF (K3.EQ.1) YR(4)=ATAN(AV*0.4*(ABS(FXOD)**(-0.6)))
    IF (K3.EQ.-1) YR(4)=-ATAN(AV*0.4*(ABS(FXOD)**(-0.6)))
    YR(3)=UV-UR+COS(YR(4))
    YR(4)=0.0
46 YR(6)=-YR(6)
    RETURN
    END
    SUBROUTINE COEF(VELO,EYCOEF,EZCOEF,DC,WC,TPER,EXNF,EYNF,EZNF,
1 EXIF,EYIF,EXFF
    VELDC=ABS(VELO)
    IF (EYCOEF.GE.0.5.AND.EYCOEF.LE.0.7) GO TO 10
    RH=(WC*DC)/(2.0*DC+WC)
    UPRINF=0.03426*VELOC/(RH**0.166667)
    EYNF=EYCOEF*DC*UPRINF
    EZNF=EZCOEF*DC*UPRINF
    EXIF=5.93*DC*UPRINF*(1.0+((EZNF*TPER/(DC**2.0))/
1 (2.0*((2.4674+((EZNF*TPER)/(DC**2.0)**2.0)**0.5))**0.5)))
    EXNF=EYNF*10.
    EYIF=EYNF
    EXFF=0.18*((VELOC*UPRINF)**0.5)*(WC**2.0)/RH*(1.0+((EZNF
1 *TPER/(DC**2.0))/((2.0*((2.4674+((EZNF*TPER)/(DC**2.0)**2.0))
2**0.5))**0.5)))
    GO TO 20
10 RH=(WC*DC)/(2.0*DC+WC)
    UPRINF=0.0952*VELOC/(RH**0.166667)
    EYIF=EYCOEF*DC*UPRINF
    EZNF=EZCOEF*DC*UPRINF
    EXIF=5.93*DC*UPRINF*(1.0+((EZNF*TPER/(DC**2.0))/
1 (2.0*((2.4674+((EZNF*TPER)/(DC**2.0)**2.0)**0.5))**0.5)))
    EXNF=EYNF*10.
    EYIF=EYNF
    EXFF=0.18*((VELOC*UPRINF)**0.5)*(WC**2.0)/RH*(1.0+((EZNF
1 *TPER/(DC**2.0))/((2.0*((2.4674+((EZNF*TPER)/(DC**2.0)**2.0))
2**0.5))**0.5)))
20 CONTINUE
    RETURN
    END

```

C *****PROGRAM TIDAL*****
C
C THIS PROGRAM CALCULATES THE PLUME TRAJECTORY AND PLUME CONCEN-
C TRATION OF A LIQUID CHEMICAL CONTINUOUSLY SPILLED INTO A BODY OF
C WATER HAVING FLUCTUATING (TIDAL) VELOCITY.
C
C INPUT FILE NAMES: TIDEIN.DAT
C OUTPUT FILE NAMES: SPILLOUT.DAT
C
C SUBROUTINE TIDAL
C
C INPUT VARIABLES:
C
C X = STARTING VALUE OF PLUME PATH INTEGRATION, M
C H = INTEGRATION STEP SIZE, M
C DISTA = INITIAL DOWNSTREAM DISTANCE TO THE FIRST PRINTOUT, M
C DISTAN = INCREMENTAL DOWNSTREAM DISTANCE BETWEEN PRINTOUTS, M
C K4 = PARAMETER TO ALLOW DEFAULT VALUES TO BE USED FOR X,
C H, DISTA, AND DISTAN. K4=1 WILL ALLOW USER INPUT.
C K4=2 WILL USE DEFAULT VALUES AND USER INPUT IS NOT
C NEEDED.
C ROA = WATER DENSITY, KG/M**3
C DENS = CHEMICAL SPILL DENSITY, KG/M**3
C ACCLASS(J) = FLOW REGIME DESCRIPTION
C DIAJET = INITIAL PLUME DIAMETER, CM
C TESTNO = EXPERIMENTAL TEST NUMBER
C QINIT = CHEMICAL DISCHARGE FLOWRATE, M**3/S
C SPTIMF = TOTAL TIME OF SPILL DISCHARGE, S
C TIMINC = TIME INCREMENT FOR COMPUTING CONCENTRATION AT OBSERVATION
C POINT, S
C TIMMAX = MAXIMUM TIME FOR COMPUTING CONCENTRATION AT OBSERVATION
C POINT, S
C TPER = TIDAL PERIOD, S
C WC = WIDTH OF THE CHANNEL, M
C DC = DEPTH OF THE CHANNEL, M
C XOBS = DOWNSTREAM DISTANCE TO THE OBSERVATION POINT, M
C YOBS = Y DIMENSION FROM THE CENTER OF THE CHANNEL TO THE
C OBSERVATION LOCATION, M
C ZOBS = Z DIMENSION FROM THE CHANNEL SURFACE TO THE OBSERVATION
C LOCATION, M (FOR THE PLUME CENTERLINE CONCENTRATION, SET
C ZOBS=-1.0)
C ALOC = DISTANCE IN THE Y DIRECTION FROM THE CHANNEL CENTERLINE TO
C THE SPILL ORIGIN, M
C BLOC = VERTICAL DISTANCE FROM THE CHANNEL SURFACE TO THE SPILL
C ORIGIN, M
C EYCOEF = Y DIFFUSION COEFFICIENT FOR THE NEAR FIELD MODEL
C EZCOEF = Z DIFFUSION COEFFICIENT FOR THE NEAR FIELD MODEL
C VNUM = ROUGHNESS FACTOR FOR FRICTION VELOCITY
C K5 = PARAMETER TO ALLOW DEFAULT VALUES TO BE USED FOR
C EYCOEF, EZCOEF, AND VNUM. K5=1 WILL ALLOW USER
C INPUT. K5=2 WILL USE DEFAULT VALUES AND USER
C INPUT IS NOT NEEDED.
C U1NF = MEAN RIVER VELOCITY, M/S
C U2NF = MAXIMUM FLUCTUATING VELOCITY OF A TIDAL RIVER, M/S
C ALFANF = PHASE SHIFT FOR THE TIDAL RIVER PERIOD, SECONDS
C K1 = INITIAL JET DIRECTION INDICATOR(+1=HORIZONTAL DOWNSTREAM,
C -1=HORIZONTAL UPSTREAM, 0=ALL OTHER CONDITIONS)
C K2 = INITIAL JET DIRECTION INDICATOR(+1=VERTICAL UPWARD, -1=V
C ERTICAL DOWNWARD, 0=ALL OTHER CASES)
C K3 = INITIAL JET DIRECTION INDICATOR(+1=HORIZONTAL TRANSVERSE
C TO THE RIGHT, -1=HORIZONTAL TRANSVERSE TO THE LEFT, 0=ALL OTHER CASES)

```

C
C DIMENSIONS:
C
C INTEGER COUNT, RUNGE, HAMING
C REAL KNF, KIF, KFF, LAM, MASS, LOC, JAY
C DOUBLE PRECISION ACLASS(4), TESTNO(1)
C DIMENSION TE(6), YR(6), FR(6), Y(4,6), F(3,6), YRS(6), LOC(5,2), ZZO(6)
C DIMENSION TRD(6,7), TJ(100), TJPR(300,3)
C DIMENSION XOD(10), ZOD(10), PATHL(10)
C COMMON/PHYS/DCDR, EPS, UPRI, ROA, DENS, G, UR
C COMMON/COND/ROT, ALFA1, ALFA2, ALFA3
C OPEN (UNIT=1, NAME='SY0:TIDEIN.DAT', 0, TYPE='OLD')
C Q-9. 80665
C N-6
C
C READ IN PARAMETERS AND INITIAL CONDITIONS.
C
C READ (1,114) DIAJET
C READ (1,123) K4
C X=0.0
C H=0.1*DIAJET
C DISTA=0.0
C DISTAN=5.*DIAJET
C IF (K4.EQ.2) GO TO 1001
C READ(1,100) X,H
C READ(1,102) DISTA,DISTAN
1001 READ(1,101) ROA,DENS
C READ(1,111) (ACCLASS(J),J=1,4)
C READ(1,115) TESTNO(1)
C READ(1,117) QINIT,SPTIME, TIMINC, TIMMAX, TPER
C READ(1,118) WC, DC
C READ(1,120) X0BS, Y0BS, Z0BS, ALOC, BLOC
C READ (1,123) K5
C EYCOEF=0.6
C EZCOEF=0.057
C VNUM=0.025
C IF (K5.EQ.2) GO TO 1002
C READ(1,121) EYCOEF, EZCOEF, VNUM
1002 READ(1,122) U1NF, U2NF, ALFANF, K1, K2, K3
C UR=U1NF
C
C PRINT PARAMETERS, HEADINGS, AND INITIAL CONDITIONS.
C
C WRITE(3,218)
C WRITE(3,203) TESTNO(1)
C WRITE(3,209) (ACLAES(J),J=1,4)
C WRITE(3,204) DISTA,DISTAN
C WRITE(3,236) ROA,DENS,DIAJET
C WRITE(3,205) QINIT,TPER,SPTIME,TIMINC,TIMMAX,WC,DC
C WRITE(3,206) ALOC,BLOC
C WRITE(3,212) U1NF,U2NF,ALFANF
C IF (K1.EQ.1) WRITE(3,251)
C IF (K1.EQ.-1) WRITE(3,252)
C IF (K2.EQ.1) WRITE(3,253)
C IF (K2.EQ.-1) WRITE(3,254)
C IF (K3.EQ.1) WRITE(3,255)
C IF (K3.EQ.-1) WRITE(3,256)
C WRITE(3,235) EYCOEF,EZCOEF
C
C THIS ROUTINE DETERMINES THE CONCENTRATION AT A GIVEN OBSERVATION
C POINT FOR A CONTINUOUS SPILL IN A TIDAL RIVER.
C
C SET MASS DECAY COEFFICIENTS TO ZERO

```

```

      KNH=0. 0
      KIF=0. 0
      KFF=0. 0
C      COMPUTE TURBULENCE LEVEL
      TLV=3. 807*VNUM/((DC*WC/(2. *DC+WC))**0. 166666)
C      FIX OGMS MODEL COEFFICIENTS
      ALFA1=0. 092
      ALFA2=1. 050
      ALFA3=1. 0
      LAM=1. 1619
      CONC=. 3679
C
C      NOW INITIALIZE TRD AND ZZO (TO BE DEFINED LATER)
      1 DO 60 I=1,6
      DO 61 J=1,7
      61 TRD(I, J)=0. 0
      ZZO(I)=0. 0
      60 CONTINUE
C
C      DIVIDE THE TIDAL PERIOD INTO SIX INCREMENTS AND CALCULATE AN AVERAGE
C      VELOCITY FOR EACH INCREMENT.
C      TRD(J, 1), J=1 TO 6, ARE THE 6 AVERAGE RIVER VELOCITIES
C
      TINV=TPER/6. 0
      DO 3 NO=1,6
      3 TRD(NO, 1)=(1. 0/TINV)*((U1NF*TINV)-((U2NF*TPER/6. 2832)*(COS((6. 2832
      1/TPER)*(TINV*NO+ALFANF))-COS((6. 2832/TPER)*(TINV)*(NO-1)+ALFANF))
      2))
C
C      CALCULATE THE CONVERSION POINTS BETWEEN THE VARIOUS FLOW REGIMES
C      FOR ALL SIX TIDAL SEGMENTS.
C      FIRST CALCULATE THE POINT OF CONVERSION FROM THE VERY NEAR FIELD
C      TO THE NEAR FIELD MODEL FOR EACH INCREMENT OF THE TIDAL CYCLE.
C
C      ****
C      STATEMENTS 4 TO 40 ARE OGMS MODEL
C
      4 HH H
      XX=X
      DO 16 NOO=1,6
      DDISTA=DISTA
      IF (TRD(NOO, 1). LT. 0. 0) NSIGN=1
      IF (TRD(NOO, 1). GE. 0. 0) NSIGN=0
      IF (TRD(NOO, 1). LT. 0. 0) TRD(NOO, 1)=-TRD(NOO, 1)
      ALTL=ALFA3*TLV
      IF (ALTL. NE. 0. 0) GO TO 18
      KWRITE(3, 232)
      GO TO 1000
      18 UPRI=TRD(NOO, 1)*TLV
      UA=TRD(NOO, 1)
      UR=TRD(NOO, 1)
      IF (ROA. EQ. DENS) DCDR=1. 0E+20
      IF (ROA. EQ. DENS) GO TO 19
      DCDR=1. 0/(1. 0-ROA/DENS)
      19 ROT=(1. 0-ROA/DENS)/ROA
      MASS=QINIT*DENS
      RATWD WC/DC
      XEND=TRD(NOO, 1)*SPTIME
      RH=(NC*DC)/(2. 0*DC+WC)
      IF (RATWD. LT. 100. 0) RH=DC
C
C      COMPUTE DIFFUSION AND DISPERSION COEFFICIENTS
C

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```

      CALL COEF (TRD(NOD, 1), EYCOEF, EZCOEF, DC, WC, TPER, EXNF, EYNF, EZNF,
1 EXIF, EYIF, EXFF)
      WRITE(3,226)
      WRITE(3,211)
      KK1=K1
      KK2=X2
      KK3=X3
38 DO 37 I=1,6
37 YR(I)=0.0
      YR(1)=DFNS
      X=XX
      CALL JET(YR, UR, QINIT, DIAJET, ROA, KK1, KK2, KK3, ALOC, BLOC, DC)
      YR2=YR(2)
      YR3=YR(3)
      YR4=YR(4)
      YR5=YR(5)
      YR6=YR(6)
      IF (YR(1).GT.0.95*DENS) YR(1)=0.95*DENS
      DO 17 NNO=1,6
      TE(NNO)=0.0
      FR(NNO)=0.0
      Y(1,NNO)=0.0
      Y(2,NNO)=0.0
      Y(3,NNO)=0.0
      Y(4,NNO)=0.0
      F(1,NNO)=0.0
      F(2,NNO)=0.0
      F(3,NNO)=0.0
17 YRS(NNO)=0.0
      EPS=0.0000000001
      COUNT=0
      IF (KK2.NE.0) H=2.5*HH*(1.0-(DENS-ROA)/ROA*KK2)*((ABS(YR(3))*1
1 (TRD(NOD, 1)**2.0)**0.5)/((U1NF+U2NF)**1.5))
      IF (KK2.EQ.0) H=HH
      AH=H
      DO 21 J=1,N
      TE(J)=0.0
21 Y(4,J)=YR(J)
22 IF (RUNGE(N,YR,FR,X,H).NE.1) GO TO 24
      CALL RHS(YR,YRS)
      DO 23 K=1,4
23 FR(K)=YRS(K)
      FR(5)=COS(YR(4))
      FR(6)=SIN(YR(4))
      GO TO 22
24 COUNT=COUNT+1
      ISUB=4-COUNT
      DO 25 J=1,N
25 Y(ISUB,J)=YR(J)
      CALL RHS(YR,YRS)
      DO 26 K=1,4
26 F(ISUB,K)=YRS(K)
      F(ISUB,5)=COS(YR(4))
      F(ISUB,6)=SIN(YR(4))
27 CONTINUE
      IF (COUNT.LE.3) GO TO 28
      IF (ABS(Y(1,1)).LT.DENS/3.0) H=AMAX1(HH,H)
      IF ((DENS-ROA)*KK2.GT.0.0.AND.Y(1,1).GT.DENS) GO TO 39
      IF ((DENS-ROA)*KK2.GT.0.0.AND.Y(1,1).LT.0.0) GO TO 39
C
C      THE ABOVE 2 STATEMENTS CHANGE THE INITIAL DIRECTION OF THE
C      DISCHARGE JET BECAUSE THE PLUME BENDS BACK ON ITSELF.
C

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```

      GO TO 31
39  KK1=1
    KK2=0
    WRITE(3,215) N00
    GO TO 38
31  IF (Y(1,5).GE.DDISTA) WRITE(3,234) Y(1,5),-Y(1,6),Y(1,1)
    IF (Y(1,5).GE.DDISTA) DDISTA=DDISTA+DISTAN
    RC=LAM*Y(1,2)*(-ALOC(0CONC))*#0.5
    IF (2.0*RC.GT.DC+Y(1,6)) GO TO 29
    IF (2.0*RC.GT.-Y(1,6)) GO TO 29
    IF (2.0*RC.GT.((WC/2.0)-ABS(ALOC))) GO TO 29
    IF (Y(1,1).LT.0.00001*DENS) GO TO 29
28  IF (Y(1,5).GT.XEND) GO TO 29
    IF (COUNT.LT.3) GO TO 22
30  M=HAMING(N,Y,F,X,H,TE)
    DO 32 K=1,4
32  YR(K)=Y(1,K)
    CALL RHS(YR,YRS)
    DO 33 K=1,4
33  F(1,K)=YRS(K)
    F(1,5)=COS(Y(1,4))
    F(1,6)=SIN(Y(1,4))
    IF (M.EQ.1) GO TO 30
    COUNT=COUNT+1
C
C      CHECK TO DETERMINE IF THE PLUME HAS INTERSECTED A CHANNEL BOUNDARY.
C      IF SO, THEN CONVERT TO A NEAR FIELD MODEL.
C
      IF (Y(1,6).GT.0.0) GO TO 29
      IF (Y(1,6).LT.-DC) GO TO 29
      GO TO 27
C
C      *****1*****X*****2*****X*****3*****
C
C      TRD(J,2), J=1 TO 6, ARE THE DOWNSTREAM ENDPOINT DISTANCES OF
C      COMS PLUMES
C
29  TRD(N00,2)=Y(1,5)
    WRITE(3,234) Y(1,5),-Y(1,6),Y(1,1)
    IF (NSIGN.EQ.1) TRD(N00,1)=-TRD(N00,2)
    WRITE(3,216)
    WRITE(3,210) TRD(N00,1),DENS,YR2,YR3,YR4,YR5,-YR6
    WRITE(3,217)
    WRITE(3,210) TRD(N00,1),DENS,YR(2),YR(3),YR(4),Y(1,5),-Y(1,6)
    IF (NSIGN.EQ.1) TRD(N00,1)=-TRD(N00,2)
    WRITE(3,214) XX,AH,H
    WRITE(3,227) EXNF,EYNF,EZNF,EXIF,EYIF,EXFF
    WRITE(3,225) AI TL
C
C      TRD(J,3), J=1 TO 6, ARE THE CENTERLINE PLUME CONCENTRATIONS
C      AT THE ENDPOINTS
C
      TRD(N00,3)=Y(1,1)
      IF (Y(1,6).GT.0.0) Y(1,6)=0.0
      IF (Y(1,6).LT.-DC) Y(1,6)=-DC
C
C      ZZO(J), J=1 TO 6, ARE THE DEPTHS OF THE PLUME ENDPOINTS
C
      IF (Z0BS.NE.-1.0) ZZO(N00)=Z0BS
      IF (Z0BS.NE.-1.0) GO TO 35
      IF (Y(1,6).EQ.0.0) ZZO(N00)=0.0
      IF (Y(1,6).EQ.-DC) ZZO(N00)=DC
40  IF (Y(1,6).NE.0.0.AND.Y(1,6).NE.-DC) ZZO(N00)=-Y(1,6)

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C
C ***** *****
C MATCH THE VERY NEAR FIELD AND NEAR FIELD MODELS AT THE POINT OF
C CONVERSION.
C
C XSTART=DOWNSTREAM LENGTH OF POINT SOURCE MODEL AT WHICH THE
C CONCENTRATION IS THE SAME AS 00MS PLUME
C
35 XSTART=((LAM*LAM)*(Y(1,2)*Y(1,2))*TRD(NOO,1))/(4.0*(EYNF*EZNF))
1<*0.5)
TRD(NOO,4)=XSTART-TRD(NOO,2)

C
C TRD(J,4), J 1 TO 6, IS THE DISTANCE UPSTREAM FROM X=0 TO THE
C VIRTUAL ORIGIN OF THE POINT SOURCE MODEL
C **** ****
C CALCULATE THE DOWNSTREAM LOCATION FOR THE POINT OF CONVERSION
C FROM THE NEAR FIELD TO THE INTERMEDIATE FIELD MODEL.
C
C TRD(J,5) IS TOTAL LENGTH OF POINT SOURCE MODEL FROM ITS
C VIRTUAL ORIGIN
C
41 TRD(NOO,5)=0.3+TRD(NOO,1)*DC*DC/EZNF
LOC(1,1)=ALOC
LOC(2,1)=WC-ALOC
LOC(3,1)=ALOC
LOC(4,1)=-WC-ALOC
LOC(5,1)=ALOC
50 LOC(1,2)=-Y(1,6)
LOC(2,2)=-Y(1,6)
LOC(3,2)=2.0*DC+Y(1,6)
LOC(4,2)=-Y(1,6)
LOC(5,2)=Y(1,6)

C
C ***** *****
C MATCH THE NEAR FIELD AND INTERMEDIATE FIELD MODELS.
C
C DETERMINE THE INITIAL CONCENTRATION FOR THE INTERMEDIATE FIELD
C MODEL BY COMPUTING THE AVERAGE POINT SOURCE CONCENTRATION OVER
C THE DEPTH AT X=TRD(J,5). USE 100 DEPTH INCREMENTS.
C
135 AVOC=0.0
DIV=DC/99.0

C
C 1/F1, 1.F2, AND 1.F3 ARE THE 3 POSSIBILITIES FOR THE LEADING
C TERM IN THE POINT SOURCE MODEL. F2 OR F3 MAY BE NEEDED
C IF THE RIVER VELOCITY IS VERY SMALL.
C
F1=12.5664*TRD(NOO,5)*((EYNF*EZNF)**0.5)/MASS
F2=44.5466*(TRD(NOO,5)**1.25)*(U2NF**0.5)*(EXNF**0.25)*
1*((EYNF*EZNF)**0.5)*(((COS(6.2832*((2*NOO-1)*TPER/2.0+ALFANF)
2/TPER)**2)**0.25)/(2.6*MASS*(TPER**0.5)*((TRD(NOO,1)**2)**0.625))
F3=44.5466*(TRD(NOO,5)**1.3333)*(U2NF**0.3333)*(EXNF**0.16667)
1*((EYNF*EZNF)**0.5)*(((SIN(6.2832*((2*NOO-1)*TPER/2.0+ALFANF)
2/TPER)**2)**0.25)/(1.86*MASS*(TPER**0.16667)*((TRD(NOO,1)**2)
3*0.6667))
IF (F1.GE.F2.AND.F1.GE.F3) F22=1.0/F1
IF (F2.GE.F1.AND.F2.GE.F3) F22=1.0/F2
IF (F3.GE.F1.AND.F3.GE.F2) F22=1.0/F3
F22=1.0/F1
IF (KNF.EQ.0.0) F23=1.0
IF (KNF.EQ.0.0) GO TO 134
IF (KNF.NE.0.0.AND.TRD(NOO,1)/(KNF*TRD(NOO,5)).GT.0.012)
1 F23=EXP(-KNF*TRD(NOO,5)/TRD(NOO,1))

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        IF (KNF.NE.0.0.AND.TRD(NOO,1)/((KNF*TRD(NOO,5)).LE.0.012)
1 F23=0.0
134 DO 136 I=1,100
      AAAZ=0.0
      VID=DIV*(I-1)
      DO 137 J=1,5
      AAAZ=EXP((-TRD(NOO,1)*((ALOC-LOC(J,1))*(ALOC-LOC(J,1)))/(4.0*
1 (TRD(NOO,5)*EYNF))-(TRD(NOO,1)*((VID-
2 LOC(J,2))*(VID-LOC(J,2)))/(4.0*(TRD(NOO,5)
3)*EZNF)))
137 AAAZ=AAA2+AAZZ
      C11I=F22+F23*AAA2
136 AVGC=AVGC/C11I
      TRD(NOO,6)=AVGC/100.0
C
C      TRD(J,6) IS THE AVERAGE CONCENTRATION
C
C      CALCULATE THE ORIGIN LOCATION IN THE X DIRECTION FOR THE FAR FIELD
C      FIELD MODEL BY GUESSING A LENGTH FROM X=0 THAT WILL GIVE A
C      CONCENTRATION EQUAL TO TRD(J,6).
C
150 MN=0
      XLSINC=0.01*TRD(NOO,5)
C
C      XLSINC IS THE INCREMENT TO THE GUESSED LENGTH.
C
      XXLS=XLSINC
144 C11IFF=0.0
      C11IF=0.0
      DO 138 I=1,20
      DII=I
C
C      1/F1, 1/F2, AND 1.F3 ARE THE 3 POSSIBILITIES FOR THE
C      LEADING TERM1 IN THE LINF SOURCE MODEL
C
      F1=(WC**2.0)*TRD(NOO,1)/((DII**2)*9.8696*EYIF*XXLS)
      IF (F1.LE.0.012) F2=0.0
      IF (F1.GT.0.012) F2=EXP(-1.0/F1)
      C11IFF=((COS(DII*3.1416*(ALOC+(WC/2.0))/WC)**2.0)*F2
138 C11IFF=C11IFF+C11IFF
      C11IFF=C11IFF*2.0+1.0
      F3=WC*DC*TRD(NOO,1)/MASS
      EXBAR=EXIF*(1.0+((EZNF*TPER/(DC**2.0))/(2.0*(2.4674+
1 ((EZNF*TPER/(DC**2.0)**2.0)**0.5))))
C
C      EXBAR IS THE TIME-AVERAGE DISPERSION COEFFICIENT
C
      F4=3.5449*WC*DC*((XXLS*TRD(NOO,1))**0.25)*(EXBAR**0.25)
      1*(ABS(COS(6.2832*((2.0*NOO-1)*TPER/2.0+ALFANF)/TPER))**0.5)/
      2(2.6*MASS*(TPER**0.5))
      F5=2.54*WC*DC*(XXLS**0.3333)*(EXBAR**0.3333)*
      1*(ABS(SIN(6.2832*((2.0*NOO-1)*TPER/2.0+ALFANF)/TPER))**0.5)/
      2(1.86*MASS*(TPER**0.6667))
      IF (F3.GE.F4.AND.F3.GE.F5) F22=1.0/F3
      IF (F4.GE.F3.AND.F4.GE.F5) F22=1.0/F4
      IF (F5.GE.F3.AND.F5.GE.F4) F22=1.0/F5
      IF (KIF.EQ.0.0) F23=1.0
      IF (KIF.EQ.0.0) GO TO 145
      IF (KIF.NE.0.0.AND.TRD(NOO,1)/((KIF*XXLS).GT.0.012)
1 F23=EXP(-KIF*XXLS/TRD(NOO,1))
      IF (KIF.NE.0.0.AND.TRD(NOO,1)/((KIF*XXLS).LE.0.012)
1 F23=0.0
145 C11IF=C11IFF*F22*F23

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RAIFNF=C11IF/TRD(NOO, 6)
IF (MN, EQ. 1) GO TO 141
IF (MN, EQ. 2) GO TO 142
IF (RAIFNF, EQ. 1.0) GO TO 16
IF (RAIFNF, LT. 1.0) MN=1
IF (RAIFNF, LT. 1.0) GO TO 141
IF (RAIFNF, GT. 1.0) MN=2
GO TO 142
141 IF (RAIFNF, LT. 0.99) XXLS=XXLS-XLSINC
IF (RAIFNF, LT. 0.99) GO TO 144
GO TO 14
142 IF (RAIFNF, GT. 1.01) XXLS=XXLS+XLSINC
IF (RAIFNF, GT. 1.01) GO TO 144
14 IF (NSIGN, EQ. 1) TRD(NOO, 1)=-TRD(NOO, 1)
TRD(NOO, 7)=XXLS-TRD(NOO, 5)+TRD(NOO, 4)

C      TRD(J, 7) IS THE UPSTREAM VIRTUAL ORIGIN FROM X=0 OF THE
C      INTERMEDIATE FIELD
C
800 TRD(NOO, 5)=TRD(NOO, 5)-TRD(NOO, 4)

C      TRD(J, 5) IS NOW THE APPLICABLE LENGTH OF THE POINT SOURCE
C      MODEL MEASURED FROM X=0.
C
16 CONTINUE
*****  

C      ALL MODELS HAVE NOW BEEN MATCHED
*****  

C
C      CALCULATE THE CONCENTRATION AS A FUNCTION OF TIME AT THE OBSERVA-
C      TION POINT.
C
990 TYPE *, 'INPUT THE OBSERVATION COORDINATES (IN METERS)'
TYPE *, 'TO TERMINATE THE RUN, ENTER XOBS=-1.0'
TYPE *, '  

TYPE *, 'INPUT XOBS'
ACCEPT *, XOBS
TYPE *, '  

TYPE *, 'INPUT YOBS'
ACCEPT *, YOBS
TYPE *, '  

TYPE *, 'INPUT ZOBS'
TYPE *, 'INPUT ZOBS=-1.0 TO OBTAIN THE CENTERLINE OF THE PLUME'
ACCEPT *, ZOBS
TYPE *, '  

IF (XOBS, EQ. -1.0) GO TO 1000
IF (ZOBS, EQ. -1.0) WRITE(3, 239) XOBS, YOBS
999 IF (ZOBS, NE -1.0) WRITE(3, 240) XOBS, YOBS

C      ****
C      DETERMINE THE RIVER VELOCITY AT THE OBSERVATION TIME
C      =TIMEE. STATEMENTS 160-261 DETERMINE WHICH OF THE TIDAL
C      SEGMENTS APPLY.
C
TIMEE=0.0
160 IAQ=0

C      A RETURN WILL BE MADE TO 160 WITH THE NEXT OBSERVATION TIME
C      AT THE COMPLETION OF THIS CYCLE OF COMPUTATIONS.
C
TMI=TIMEE/TPER
161 IF (TMI, GT. 1.0) IAQ=IAQ+1
IF (TMI, GT. 1.0) TMI=TMI-1.0

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        IF (TMI.GT.1.0) GO TO 161
C
C      IAG IS THE NUMBER OF TIDAL CYCLES < OR = TIMEE.
C
C      IF (TMI.LT.1.0/6.0) IKM=1
C
C      IKM IS THE NUMBER OF THE TIDAL SEGMENT OF INTEREST.
C
C      IF (TMI.LT.1.0/3.0 AND. TMI.GE.1.0/6.0) IKM=2
C      IF (TMI.LT.1.0/2.0 AND. TMI.GE.1.0/3.0) IKM=3
C      IF (TMI.LT.2.0/3.0 AND. TMI.GE.1.0/2.0) IKM=4
C      IF (TMI.LT.3.0/6.0 AND. TMI.GE.2.0/3.0) IKM=5
261 IF (TMI.GE.5.0/6.0) IKM=6
C
C      SOLVE THE EQUATIONS FOR DETERMINING
C      THE NUMBER OF TIMES THE WATER NOW AT THE OBSERVATION
C      POINT HAS PASSED UNDER THE SPILL ORIGIN.
C      STATEMENTS 600-616 DO THIS BY A MODIFIED NEWTONS ROOT-
C      SOLVING METHOD.
C
C      600 NCYC=1
C          IK4=1
C          ICOUNT=0
C          DO 610 I=1,300
C          DO 610 J=1,3
610 TJPR(I,J)=0.0
611 TJPR(NCYC,2)=XOBS-U1NF*TIMEE+((U2NF*TPER)/6.2832)*(COS(6.2832/
1TPER*(TIMEE+ALFANF)))+U1NF*TJPR(NCYC,1)-((U2NF*TPER)/6.2832)*
2(COS(6.2832/TPER*(TJPR(NCYC,1)+ALFANF)))
C
C      THE ROOT CORRESPONDS TO TJ(NCYC,2)=0
C
C      TJPR(NCYC,3)=U1NF+U2NF*(SIN(6.2832/TPER*(TJPR(NCYC,1)+ALFANF)))
C
C      TJ(NCYC,3) IS THE RIVER VELOCITY AT GUESSED ROOT TIME TJ(NCYC,1)
C
C      IF (NCYC.EQ.1) GO TO 608
C      IF (IKA.GT.1) GO TO 608
C      IF ((TJPR(NCYC,3)-TJPR(NCYC-1,3)).LE.0.0 AND. (TJPR(NCYC,2)*
1TJPR(NCYC-1,2)).GT.0.0) IKA=10
C          IF (IKA.GT.1) NCYC=NCYC-1
C          IF (ICOUNT.EQ.10) GO TO 700
C          GO TO 608
700 ICOUNT=0
C          IK4=1
608 IF (TJPR(NCYC,1).EQ.TIMEE) NCYC=NCYC+1
C          IF (TJPR(NCYC-1,1).EQ.TIMEE) GO TO 622
C          NCYC=NCYC+1
C          IF (NCYC.GT.300) TYPE *, 'NCYC EXCEEDS 300. RUN TERMINATED.'
C          IF (NCYC.GT.300) WRITE(3,250)
C          IF (NCYC.GT.300) GO TO 1000
C          TJPR(NCYC,1)=TJPR(NCYC-1,1)+TPER/(2.0*IKA)
C          IF (IKA.GT.1) ICOUNT=ICOUNT+1
C          IF (TJPR(NCYC,1).LE.TIMEE) GO TO 611
C          TJPR(NCYC,1)=TIMEE
C          GO TO 611
622 NCYC=NCYC-1
C          NRTJ=0
C          NIT=1
612 IF (TJPR(NIT,2).LT.0.0) GO TO 613
C          IF (TJPR(NIT,2).GE.0.0) GO TO 614
613 NIT=NIT+1
C          IF (NIT.GT.NCYC) GO TO 616

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        IF (TJPR(NIT,2). LT. 0.0) GO TO 613
        NIT=NIT-1
        GO TO 615
614  NIT=NIT+1
        IF (NIT. GT. NCYC) GO TO 616
        IF (TJPR(NIT,2). GE. 0.0) GO TO 614
        NIT=NIT-1
615  FROT11=TJPR(NIT,2)
        FROT22=TJPR(NIT+1,2)
        TROT11=TJPR(NIT,1)
        TROT22=TJPR(NIT+1,1)
617  TROOT1=TROT11+((ABS(FROT11))*(TROT22-TROT11))/(ABS(FROT11)
1+ABS(FROT22))
        FROOT1=XOBS-U1NF*TIMEE+((U2NF*TPER)/6. 2832)*(COS(6. 2832/TPER
1*(TIMEE+ALFANF)))+U1NF*TROOT1-((U2NF*TPER)/6. 2832)*(COS(6. 2832
2/TPER*(TROOT1+ALFANF)))
        IF (ARS(FROOT1). LE. 0.01) GO TO 619
        IF ((FROT11/FROOT1). LE. 0.0) GO TO 640
        ZZ=ABS(FROOT1)/(ABS(FROOT1)+ABS(FROT22))
        TTROT2=TROT22
        GO TO 641
640  ZZ=ABS(FROOT1)/(ABS(FROOT1)+ABS(FROT11))
        TTROT2=TROT11
641  TROOT2=TROT1+ZZ*(TTROT2-TROOT1)
        TFROT2=XOBS-U1NF*(TIMEE-TROOT2)+((U2NF*TPER)/6. 2832)*
1((COS(6. 2832/TPER*(TIMEE+ALFANF)))-(COS(6. 2832/TPER*
2(TROT2+ALFANF)))
        IF ((TFROT2/FROOT1). GE. 0.0. AND. (TROOT2/TROOT1). GE. 1.0)
1TROT11=TROOT2
        IF ((TFROT2/FROOT1). GE. 0.0. AND. (TROOT2/TROOT1). LT. 1.0)
1TROT22=TROOT2
        IF ((TFROT2/FROOT1). LT. 0.0. AND. (TROOT2/TROOT1). GE. 1.0)
1TROT11=TROOT1
        IF ((TFROT2/FROOT1). LT. 0.0. AND. (TROOT2/TROOT1). GE. 1.0)
1TROT22=TROOT2
        IF ((TFROT2/FROOT1). LT. 0.0. AND. (TROOT2/TROOT1). LT. 1.0)
1TROT11=TROOT2
        IF ((TFROT2/FROOT1). LT. 0.0. AND. (TROOT2/TROOT1). LT. 1.0)
1TROT22=TROOT1
        FROT11=XOBS-U1NF*(TIMEE-TROT11)+((U2NF*TPER)/6. 2832)*
1((COS(6. 2832/TPER*(TIMEE+ALFANF)))-(COS(6. 2832/TPER*
2(TROT11+ALFANF)))
        FROT22=XOBS-U1NF*(TIMEE-TROT22)+((U2NF*TPER)/6. 2832)*
1((COS(6. 2832/TPER*(TIMEE+ALFANF)))-(COS(6. 2832/TPER*
2(TROT22+ALFANF)))
        IF (ARS(TROOT2-TROOT1). LE. (0. 00001*TPER/2.0)) GO TO 619
        GO TO 617
619  NRTJ=NRTJ+1
C
C      NRTJ IS THE NUMBER OF ROOTS AND TJ(NRTJ) ARE THE
C      CORRESPONDING ROOTS (TIMES).
C
        TJ(NRTJ)=TROOT1
        NIT=NIT+1
        GO TO 612
616  CONTINUE
        IF (NRTJ. EQ. 0) TIMEE=TIMEE+TIMINC
        IF (NRTJ. EQ. 0. AND. TIMEE. LE. TIMMAX) GO TO 160
624  IF (NRTJ. EQ. 0. AND. TIMEE. GT. TIMMAX) GO TO 1000
C
C      ***** ****
C      DETERMINE WHAT MODELS ARE REQUIRED TO CALCULATE THE CONCENTRATION
C      AT THE OBSERVATION POINT BY DETERMINING WHAT MODELS APPLY

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```

C      AT THE ROOT TIMES.
C
C      CONCEN=0. 0
C      CONVNF=0. 0
C      CONNF=0. 0
C      CONIF=0. 0
C      IVNF=0
C      INF=0
C      IIMFD=0
C
C      DETERMINE IF OBSERVATION POINT IS IN THE SPILL
C
C      KT=TIMEE/TPER
C
C      KT=INTEGER NO. OF WHOLE TIDAL PERIODS IN TIMEE
C
C      TTG=TIMEE-KT*TPER
C      AD=U1NF*KT*TPER
C
C      AD=DOWNSTREAM DISTANCE OF LEADING EDGE AFTER KT PERIODS
C
C      XEND=0. 0
C      XSTART=0. 0
C      TTG=TPER/6.
C      DO 320 J=1, 6
C      TTG=TTG-J*TPER/6.
C      IF (TTG. LT. 0. 0) TTG=TTG + J*TPER/6.
C      IF (TTG. LT. 0. 0 . AND. J . NE. 1) GO TO 321
C      IF (TRD(J, 1). LT. 0.0) GO TO 310
C      XEND=XEND+TRD(J, 1)*TTG
C      GO TO 320
C 310 XSTART=XSTART+TRD(J, 1)*TTG
C 320 CONTINUE
C 321 XEND=XEND+AD
C      IF (TIMEE. GT. SPTIME) GO TO 330
C      XSTART=XSTART
C      GO TO 340
C
C      NOW FOR TIMEE>SPTIME
C
C 330 XSTART=0. 0
C      TTG=TPER/6.
C      KT=SPTIME/TPER
C      TTG =SPTIME-KT*TPER
C      BD=U1NF*KT*TPER
C
C      BD IS DOWNSTREAM LOCATION OF TRAILING EDGE
C
C      DO 323 J=1, 6
C      TTG=TTG-J*TPER/6.
C      IF (TTG. LT. 0. 0) TTG=TTG+J*TPER/6.
C      IF (TTG. LT. 0. 0 . AND. J . NE. 1) GO TO 326
C      IF (TRD(J, 1). GT. 0.0) GO TO 325
C      XSTART=XSTART+TRD(J, 1)*TTG
C 325 CONTINUE
C 326 XSTART=XSTART+BD
C 340 IF(XOBS. GT. XEND. OR. XOBS. LT. XSTART) CONCEN=0. 0
C      IF(XOBS. GT. XEND. OR. XOBS. LT. XSTART) GO TO 350
C
C      NOW DETERMINE IF XOBS LIES IN THE MOST RECENT VERY NEAR FIELD
C
C      DO 625 I=1, NRTJ
C 625 TJPR(I, 1)=0. 0

```

```

DO 620 IEB=1, NRTJ
IYZ=NRTJ-IEB+1
IIVNF=0
IIIAQ=0
TTTMI=TJ(IYZ)/TPER

C
C THIS IS THE SAME PROCEDURE AS THE BLOCK STARTING AT 160
C BUT USES ROOT TIMES RATHER THAN TIMEE.
C

633 IF (TTTMI. OT. 1. 0) IIIAQ=IIIAQ+1
IF (TTTMI. OT. 1. 0) TTTMI=TTTMI-1. 0
IF (TTTMI. OT. 1. 0) GO TO 633
IF (TTTMI. LT. 1. 0/6. 0) IIIKM=1
IF (TTTMI. LT. 1. 0/3. 0. AND. TTTMI. GE. 1. 0/6. 0) IIIKM=2
IF (TTTMI. LT. 1. 0/2. 0. AND. TTTMI. GE. 1. 0/3. 0) IIIKM=3
IF (TTTMI. LT. 2. 0/3. 0. AND. TTTMI. GE. 1. 0/2. 0) IIIKM=4
IF (TTTMI. LT. 5. 0/6. 0. AND. TTTMI. GE. 2. 0/3. 0) IIIKM=5
IF (TTTMI. GT. 5. 0/6. 0) IIIKM=6
IF (IEB. NE. 1) GO TO 626

C
C THIS ONLY PERMITS THE MOST RECENT VERY NEAR FIELD TO
C BE CONSIDERED.
C

IF ((TRD(IIIKM, 1)/X0BS). GT. 0. 0. AND. (TRD(IIIKM, 2)/X0BS). GE. 1. 0)
IIVNF=1

C
C THE ABOVE STATEMENT INSURES THAT THE MOST RECENT VERY
C NEAR FIELD DOES OVERLIF X0BS IN BOTH MAGNITUDE AND DIRECTION
C IF IIVNF=1 THERE IS A VERY NEAR FIELD THAT CONTRIBUTES TO
C THE TOTAL CONCENTRATION
C

IF (IIVNF. EQ. 1) GO TO 620
626 IF ((TRD(IIIKM, 2)/ABS(X0BS)). GE. 1. 0) IIVNF=1

C
C THIS APPLIES WHEN RIVER VELOCITY IS IN THE OPPOSITE DIRECTION OF
C X0BS AND SU A REVERSED NEAR FIELD MUST BE USED
C

IF (IIVNF. EQ. 1) GO TO 627
IF (TRD(IIIKM, 5)/ABS(X0BS). GE. 1. 0) GO TO 627
GO TO 620
627 IJ-IIIKM
KK=0
YY=ABS(TRD(IJ, 1))*(TPER*(IIIAQ+IJ/6. 0)-TJ(IYZ))
IF ((TPER*(IIIAQ+IJ/6. 0)). EQ. TIMEE) GO TO 634
628 IF (IJ. LT. 6) GO TO 629
IJ 1
GO TO 630
629 IJ-IJ+1
630 KK=KK+1
TT=TPER*(IIIAQ+(IIIKM+KK)/6. 0)
IF (TT. LE. TIMEE) YY=YY+ABS(TRD(IJ, 1))*TPER/6. 0
IF (TT. LE. TIMEE) GO TO 628
YY=YY+ABS(TRD(IJ, 1))*(TIMEE-(TT-TPER/6. 0))
634 IF (IIVNF. EQ. 0) GO TO 631

C
C INF=NUMBER OF CONTRIBUTING NEAR FIELDS
C

TJPR(IYZ, 1)=ABS(YY-TRD(IIIKM, 2))
INF=INF+1
GO TO 620
631 IF (YY. LE. TRD(IIIKM, 5)) INF=INF+1
IF (YY. LE. TRD(IIIKM, 5)) GO TO 620
TJPR(IYZ, 1)=YY-TRD(IIIKM, 5)

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```

620 CONTINUE
NROOTS=0
IF (IVNF.NE.1) GO TO 180
C
C ****
C
C CALCULATE THE CONTRIBUTION TO THE CONCENTRATION OF THE ONE
C APPLICABLE VERY NEAR FIELD
C
158 IF (TRD(IKM, 1).GE. 0.0) NSIGN=0
IF (TRD(IKM, 1).LT. 0.0) NSIGN=1
IF (NSIGN.EQ.1) TRD(IKM, 1)=-TRD(IKM, 1)
ALTL=ALFA3*TLV
UPRI=TRD(IKM, 1)*TLV
UA=TRD(IKM, 1)
UR=TRD(IKM, 1)
IF (ROA.EQ.DENS) DCDR=1.0E+20
IF (ROA.EQ.DENS) GO TO 159
DCDR=1.0/(1.0-ROA/DENS)
159 ROT=(1.0-ROA/DENS)/ROA
RATWD=WC/DC
XEND=TRD(IKM, 1)*SPTIME
MASS=QINIT*DENS
RH=(WC*DC)/(2.0*DC+WC)
IF (RATWD.GT.100.0) RH=DC
CALL COEF(TRD(IKM, 1), EYCOEF, EZCOEF, DC, WC, TPER, EXNF, EYNF, EZNF,
1EXIF, EYIF, EXFF)
KK1=K1
KK2=K2
KK3=K3
183 DO 190 I=1,6
190 YR(I)=0.0
X=XX
YN(1)=DFNS
CALL JE1 (YR, UR, QINIT, DIAJET, RDA, KK1, KK2, KK3, ALOC, BLOC, DC)
IF (YR(1).GT.0.95*DENS) YR(1)=0.95*DENS
DO 162 I=1,6
TE(I)=0.0
FR(I)=0.0
Y(1,I)=0.0
Y(2,I)=0.0
Y(3,I)=0.0
Y(4,I)=0.0
F(1,I)=0.0
F(2,I)=0.0
F(3,I)=0.0
162 YRS(I)=0.0
EPS=0.0000000001
COUNT=0
IF (KK2.NE.0) H=2.5*HH*(1.0-(DENS-ROA)/ROA*KK2)*((ABS(YR(3))*1
1(TRD(IKM, 1)**2.0)**0.5)/((U1NF+U2NF)**1.5))
IF (KK2.EQ.0) H=HH
DO 163 J=1,N
TE(J)=0.0
163 Y(4,J)=YR(J)
165 IF (RUNGE(N, YR, FR, X, H).NE.1) GO TO 166
CALL RHS(YR, YRS)
DO 164 K=1,4
164 FR(K)=YRS(K)
FR(5)=COS(YR(4))
FR(6)=SIN(YR(4))
GO TO 165
166 COUNT=COUNT+1

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ISUB=4-COUN1
DO 167 J=1,N
167 Y(ISUB,J)=YR(J)
CALL RHS (YR, YRS)
DO 168 K=1,4
168 F(ISUB,K)=YRS(K)
F(ISUB,5)=COS(YR(4))
F(ISUB,6)=SIN(YR(4))
169 CONTINUE
IF (COUN1.LE.3) GO TO 187
IF (ABS(Y(1,1)).LT.DENS/3.0) H=AMAX1(HH,H)
IF ((DENS-ROA)*KK2.GT.0.0.AND.Y(1,1).GT.DENS) GO TO 181
IF ((DENS-ROA)*KK2.GT.0.0.AND.Y(1,1).LT.0.0) GO TO 181
GO TO 182
181 KK1=1
KKP=0
GO TO 183
182 IF (Y(1,5).GE.XOBS) GO TO 186
187 IF (COUN1.LT.3) GO TO 165
171 M-HAMINQ(N,Y,F,X,H,TE)
DO 189 K=1,4
185 YR(K)=Y(1,K)
CALL RHS(YR, YRS)
DO 172 K=1,4
172 F(1,K)=YRS(K)
F(1,5)=COS(Y(1,4))
F(1,6)=SIN(Y(1,4))
IF (M.EQ.1) GO TO 171
COUNT=COUN1+1
GO TO 169
186 IF (ZOBS.EQ.-1.0) ZZOBS=-Y(1,6)
IF (ZOBS.EQ.-1.0) GO TO 170
ZZOBS=ZOBS
170 COOM1=EXP(-((YOBS-ALOC)*(YOBS-ALOC)+(ZZOBS+Y(1,6))*(ZZOBS+Y(1,6)))
1)/((LAM*LAM)*((Y(1,2))*(Y(1,2))))
COOM2=EXP(-((YOBS-WC+ALOC)*(YOBS-WC+ALOC)+(ZZOBS+Y(1,6))*(ZZOBS+
1Y(1,6)))/((LAM*LAM)*((Y(1,2))*(Y(1,2))))
COOM3=EXP(-((YOBS-ALOC)*(YOBS-ALOC)+(ZZOBS-2.0*DC-Y(1,6))*(
1(ZZOBS-2.0*DC-Y(1,6)))/((LAM*LAM)*((Y(1,2))*(Y(1,2)))))
COOM4=EXP(-((YOBS+WC+ALOC)*(YOBS+WC+ALOC)+(ZZOBS+Y(1,6))*(ZZOBS+
1Y(1,6)))/((LAM*LAM)*((Y(1,2))*(Y(1,2))))
COOM5=EXP(-((YOBS-ALOC)*(YOBS-ALOC)+(ZZOBS-Y(1,6))*(ZZOBS-
1Y(1,6)))/((LAM*LAM)*((Y(1,2))*(Y(1,2)))))
COOM=COOM1+COOM2+COOM3+COOM4+COOM5
CONVNF=Y(1,1)*COOM
NROOTS=NROOTS+1
IF (NSIGN.EQ.1) TRD(IKM,1)=-TRD(IKM,1)
IF (NROOTS.EQ.NRTJ) GO TO 179
180 MNI=0
IF (INF.LT.1) GO TO 176
C
C ***** *****
C
C CALCULATE THE CONTRIBUTION TO THE CONCENTRATION OF ALL
C THE APPLICABLE NEAR FIELDS.
C
175 NVALU=IVNF
IAQQ=0
TMII=TJ(NRTJ-NVALU)/TPER
199 IF (TMII.GT.1.0) IAQQ=IAQQ+1
IF (TMII.GT.1.0) TMII=TMII-1.0
IF (TMII.GT.1.0) GO TO 199
IF (TMII.LT.1.0/6.0) IKM=1

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IF (TMII.LT.1.0/3.0.AND.TMII.GE.1.0/6.0) IKM=2
IF (TMII.LT.1.0/2.0.AND.TMII.GE.1.0/3.0) IKM=3
IF (TMII.LT.2.0/3.0.AND.TMII.GE.1.0/2.0) IKM=4
IF (TMII.LT.5.0/6.0.AND.TMII.GE.2.0/3.0) IKM=5
IF (TMII.GE.5.0/6.0) IKM=6
IZX=NRTJ-NVALU
UIJ1=TRD(IKM,1)
UIJ2=U1NF/U2NF*SIN(6.2832*(TJ(IZX)+ALFANF)/TPER)
IF (ARS(UTJ1).GE.ABS(UTJ2)) UTJ=UTJ1
IF (ARS(UTJ1).LT.ABS(UTJ2)) UIJ=UTJ2
UBARJ=ABS(XOBS)/(TIMEE-TJ(IZX))
CNNFS=0.0
VELO=ABS(TRD(IKM,1))
CALL COEF(VELO,EYCOEF,EZCOEF,DC,WC,TPER,EXNF,EYNF,EZNF,
1EYIF,EZIF,EXFF)
XXXOB=ABS(XOBS+TRD(IKM,4))+TJPR(IZX,1)
ZZOBS=ZZO(IKM)
F1=12.5664*XXXOB*((EYNF*EZNF)**0.5)*(ABS(UTJ))/(MASS*UBARJ)
F22=1.0/F1
DO 174 I=1,5
CNNFS=EXP(-((UBARJ*((Y0BS-LOC(I,1))*(Y0BS-LOC(I,1))))/(4.0*
1XXXOB*EYNF))-((UBARJ*((ZZOBS-LOC(I,2))*(ZZOBS-LOC(I,2))))/
2(4.0*XXXOB*EZNF)))
174 CONNFS=CONNFS+CNNFS
CONNFS=CONNFS+F22*EXP(-KNF*XXXOB/UBARJ)
CONNFS=CONNFS+CONNFS
NROOTS=NROOTS+1
IF (NROOTS.EQ.NRTJ) GO TO 179
NVALU=NVALU+1
IF ((NVALU-IVNF+1).LE.INF) GO TO 175
GO TO 176

C ****
C
C CALCULATE THE CONTRIBUTION TO THE CONCENTRATION OF ALL
C THE APPLICABLE INTERMEDIATE FIELD MODELS.
C

176 NVALU=IVNF+INF
178 IZY=NUMBER OF CONTRIBUTING INTERMEDIATE FIELD MODELS
IIAQ=0
TTMI=TJ(NRTJ-NVALU)/TPER
188 IF (TTMI.GT.1.0) IIAQ=IIAQ+1
IF (TTMI.GT.1.0) TTMI=TTMI-1.0
IF (TTMI.GT.1.0) GO TO 188
IF (TTMI.LT.1.0/6.0) IIKM=1
IF (TTMI.LT.1.0/3.0.AND.TTMI.GE.1.0/6.0) IIKM=2
IF (TTMI.LT.1.0/2.0.AND.TTMI.GE.1.0/3.0) IIKM=3
IF (TTMI.LT.2.0/3.0.AND.TTMI.GE.1.0/2.0) IIKM=4
IF (TTMI.LT.5.0/6.0.AND.TTMI.GE.2.0/3.0) IIKM=5
IF (TTMI.GT.5.0/6.0) IIKM=6
UIJ=TRD(IIKM,1)
UBARJ=ABS(XOBS)/(TIMEE-TJ(NRTJ-NVALU))
CNNIFS=0.0
CNMIF=0.0
CALL COEF(ABS(TRD(IIKM,1)),EYCOEF,EZCOEF,DC,WC,TPER,EXNF,EYNF,
1EZNF,EYIF,EXFF)
XXDIS=TRD(IIKM,7)+ABS(XOBS)+TJPR(IZX,1)
ZZOBS=ZZO(IIKM)
DO 177 I=1,20
BII=I
F1=(WC**2.0)*UBARJ/((BII**2)*9.8696*EYIF*XXDIS)
IF (F1.LE.0.012) F2=0.0

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IF (F1.GT.0.012) F2=EXP(-1.0/F1)
CNNIFS=(COS(BII*3.1416*(ALOC+(WC/2.0))/WC))*F2
1*(COS(BII*3.1416*(Y0BS+(WC/2.0))/WC))
177 CNNIF=CNNIF+CNNIFS
CNNIF=1.0+(2.0*CNNIF)
F3=WC*DC*(ARS(UTJ))/MASS
EXBAR=EXIF+(1.0+((EZNF*TPER/(DC**2.0))/(2.0*(2.4674+((EZNF*TPER/
1(DC**2.0))**2.0)**0.5))))
F4=3.5449*WC*DC*((XXDIS*
1UBARJ)**0.25)*(EXBAR**0.25)*(ABS(COS(6.2832/TPER*(TJ(NRTJ-NVALU)-
2ALFANF))**0.5)/(2.6*MASS*(TPER**0.5)))
F5=2.54*WC*DC*(XXDIS
1**0.3333)*(EXBAR**0.3333)*(ABS(SIN(6.2832/TPER*(TJ(NRTJ-NVALU)-
2ALFANF))**0.5)/(1.86*MASS*(TPER**0.6667)))
IF (F3.GE.F4.AND.F3.GE.F5) F22=1.0/F3
IF (F4.GE.F3.AND.F4.GE.F5) F22=1.0/F4
IF (F5.GE.F3.AND.F5.GE.F4) F22=1.0/F5
CONIF=CONIF+CNNIF+F22*EXP(-KIF*XXDIS/UBARJ)
NROOTS=NROOTS+1
IF (NROOTS.EQ.NRTJ) GO TO 179
NVALU=NVALU+1
GO TO 178

C
C      NOW SUM ALL THE CONTRIBUTIONS
C
179 CONCEN=CONVNF+CONNF+CONIF
350 WRITE(3,239) TIMEE, CONCEN, ZZ0BS
CONVNF=0.0
CONNF=0.0
CONIF=0.0
TIMEE=TIMEE+TIMINC
IF (TIMEE.LE.TIMMAX) GO TO 160

C
C      RETURN TO COMPUTE CONCENTRATION FOR THE NEXT TIME
C
GO TO 990

C
C      "GO TO 990" ALLOWS THE USER TO CHANGE OBSERVATION POINT
C      BUT THE SAME TIME SPAN WILL BE USED
C
C
C      FORMATS FOR INPUT AND OUTPUT STATEMENTS.
C
99 FORMAT(6X,I3)
100 FORMAT(2X,F10.4,4X,F10.6)
101 FORMAT(4X,F9.3,7X,F9.3)
102 FORMAT(6X,F12.4,9X,F12.4)
111 FORMAT(4A8)
114 FORMAT(7X,F9.4)
115 FORMAT(7X,A8)
117 FORMAT(6X,E11.4,9X,F10.1,9X,F10.1/7X,F10.1,7X,F10.1)
118 FORMAT(3X,F9.3,5X,F9.3)
120 FORMAT(5X,F10.1,7X,F10.3,7X,F10.3/5X,F10.3,7X,F10.3)
121 FORMAT(7X,F10.5,9X,F10.5,7X,F10.5)
122 FORMAT(5X,F10.2,7X,F10.2,9X,F10.4/3X,I2,5X,I2,5X,I2)
123 FORMAT(3X,I2)
204 FORMAT(6X,50HO INITIAL DOWNSTREAM DISTANCE TO FIRST PRINT
10UT = ,F12.4,2H M/6X,54HO INCREMENTAL DOWNSTREAM DISTANCE
2 BETWEEN PRINTOUTS = ,F12.4,2H M)
205 FORMAT(6X,32HO CHEMICAL DISCHARGE FLOWRATE = ,E11.4,7H M**3/S
1/6X,17HO TIDAL PERIOD = ,F14.4,8H SECONDS
2/6X,24HO TOTAL TIME OF SPILL = ,F14.4,8H SECONDS
3/6X,50HO TIME INCREMENT FOR CONCENTRATION CALCULATIONS

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4 = , F14. 4, 8H SECONDS
 5/6X, 38HO MAXIMUM TIME FOR SPILL EVALUATION = , F14. 4, 8H SECONDS
 6/6X, 21HO WIDTH OF CHANNEL = , F9. 3, 2H M
 7/6X, 21HO DEPTH OF CHANNEL = , F9. 3, 2H M)
 206 FORMAT(6X, 39HO DISTANCE FROM THE CHANNEL CENTERLINE TO THE SPILL
 1 ORIGIN/8X, 21HIN THE Y DIRECTION = , F10. 3, 2H M
 2/6X, 55HO DISTANCE FROM THE CHANNEL SURFACE TO THE SPILL ORIGIN
 3/8X, 21HIN THE Z DIRECTION = , F10. 3, 2H M)
 212 FORMAT(6X, 31HO MEAN VELOCITY OF THE RIVER = , F10. 2, 4H M/S/6X
 1, 52HO MAXIMUM FLUCTUATION VELOCITY OF THE TIDAL RIVER = , F10. 2, 4H
 2M/S/6X, 36HO PHASE SHIFT OF THE TIDAL PERIOD = , F10. 4, 8H SECONDS
 3/6X, 31HO ORIENTATION OF THE SPILL JET:)
 235 FORMAT(//4X, 46HDIFFUSION FACTORS FOR THE NEAR FIELD EQUATION: /
 1/7X, 21HO EY COEFFICIENT = , F10. 5/7X, 21HO EZ COEFFICIENT = , F10
 2. 5//)
 208 FORMAT(2X, 10HTEST NO. : , A8)
 209 FORMAT(/2X, 24HLOW FIELD DESCRIPTION: , 4A8//)
 210 FORMAT(6X, 29HO CHANNEL AVERAGE VELOCITY = ,
 1F8. 4, 4H M/S/6X, 18HO PLUME DENSITY = ,
 2F12. 5, 8H KG/M**3/6X, 32HO PLUME CHARACTERISTIC RADIUS = , F12. 5, 2H
 3 M/6X, 44HO PLUME VELOCITY (STREAM SPEED COMPONENT) = , F12. 5, 4H M/S
 4/6X, 45HO PLUME ANGLE (WITH RESPECT TO HORIZONTAL) = , F12. 5, 8H RADI
 5ANS/6X, 37HO X (HORIZONTAL DISTANCE FROM VENT) = , F12. 5, 2H
 6M/6X, 36HO Z (VERTICAL DEPTH FROM SURFACE) = , F12. 5, 2H M//)
 216 FORMAT(//4X, 18HINITIAL CONDITIONS//)
 217 FORMAT(//4X, 16HFINAL CONDITIONS//)
 211 FORMAT(//5X, 38HVERY NEAR FIELD PLUME CENTERLINE PATH:
 1//7X, 1HX, 14X, 1HZ, 10X, 17HCONCENTRATION(CL)/4X, 8H(METERS), 7X,
 28H(METERS), 10X, 9H(KG/M**3)//)
 234 FORMAT(2X, F12. 4, 3X, F12. 4, 7X, E11. 4)
 236 FORMAT(6X, 18HO WATER DENSITY = , F9. 3, 8H KG/M**3/6X,
 127HO CHEMICAL SPILL DENSITY = , F9. 3, 8H KG/M**3
 3/6X, 27HO INITIAL PLUME DIAMETER = , F9. 4, 3H CM)
 214 FORMAT(30H NUMERICAL INTEGRATION DATA//7X, 19HO STARTING
 1 POINT=, F10. 4/7X, 22HO INITIAL STEP SIZE=, F10. 6/7X, 20HO FINAL
 2 STEP SIZE=, F10. 6//)
 215 FORMAT(/2X, 34HJET DIRECTION CHANGED FOR SEGMENT , I2//)
 225 FORMAT(X, 27HALFA3 * TURBULENCE LEVEL = , F10. 5)
 226 FORMAT(1H1)
 227 FORMAT(2X, 33HTURBULENT DIFFUSION COEFFICIENTS: //7X,
 17HEXNF = , E11. 4/7X, 7HEYNF = , E11. 4/7X, 7HEZNF = , E11. 4//7X,
 27HEXIF = , E11. 4/7X, 7HEYIF = , E11. 4//7X, 7HEXFF = , E11. 4//)
 232 FORMAT(/2X, 63HTURBULENCE FACTOR MULTIPLIED BY ALFA 3 IS ZERO. RUN
 1 TERMINATED.)
 218 FORMAT(1H1, /2X, 11HTIDAL RIVER//)
 237 FORMAT(19X, F10. 1)
 238 FORMAT(1H1, 6X, 38HCONCENTRATION AT THE OBSERVATION POINT
 1//6X, 51HIE DOWNSTREAM DISTANCE TO THE OBSERVATION POINT = , F12
 2. 3, 2H M//6X, 57HTHE TRANSVERSE DISTANCE FROM THE CENTER OF THE
 3 CHANNEL TO/6X, 24HTHE OBSERVATION POINT = , F12. 3, 2H M//6X,
 448HTHE OBSERVATION POINT IS AT THE PLUME CENTERLINE
 5////23X, 4HTIME, 14X, 13HCONCENTRATION, 6X, 4HZOBS/
 621X, 9H(SECONDS), 13X, 9H(KG/M**3), 6X, 8H(METERS)//)
 239 FORMAT(19X, F10. 1, 12X, E11. 4, 3X, F12. 3)
 240 FORMAT(1H1, 6X, 38HCONCENTRATION AT THE OBSERVATION POINT
 1//6X, 51HIE DOWNSTREAM DISTANCE TO THE OBSERVATION POINT = , F12
 2. 3, 2H M//6X, 57HTHE TRANSVERSE DISTANCE FROM THE CENTER OF THE
 3 CHANNEL TO/6X, 24HTHE OBSERVATION POINT = , F12. 3, 2H M
 4////23X, 4HTIME, 14X, 13HCONCENTRATION, 6X, 4HZOBS/
 621X, 9H(SECONDS), 13X, 9H(KG/M**3), 6X, 8H(METERS)//)
 248 FORMAT(1H1)
 250 FORMAT(/3X, 33HINCYC EXCEEDS 300. RUN TERMINATED.)
 251 FORMAT(6X, 26H HORIZONTAL DOWNSTREAM)

```
252 FORMAT(6X,24H      HORIZONTAL UPSTREAM)
253 FORMAT(6X,20H      VERTICAL UPWARD)
254 FORMAT(6X,22H      VERTICAL DOWNWARD)
255 FORMAT(6X,39H      HORIZONTAL TRANSVERSE TO THE RIGHT)
256 FORMAT(6X,39H      HORIZONTAL TRANSVERSE TO THE LEFT)
270 FORMAT(1H1,2X,64HTHE TRD MATRIX CONTAINS THE MATCHING INFORMATION
1 FOR THE VARIOUS/2X, 15HTIDAL SEGMENTS. //4X, 31HTRD(I,1) = RIVER
2 VELOCITY (M/S)//4X, 63HTRD(I,2) = THE CONVERSION POINT FROM THE
3 VERY NEAR FIELD TO THE/15X, 42HNEAR FIELD IN THE STREAMWISE
4 DIRECTION (M)//4X, 55HTRD(I,3) = THE CENTERLINE CONCENTRATION AT
5 THE POINT OF/15X, 47HCONVERSION FROM THE VERY NEAR FIELD TO THE
6 NEAR/15X, 15HFIELD (KG/M**3)//4X, 60HTRD(I,4) = THE ADJUSTMENT
7 IN THE X DIRECTION AT THE POINT OF/15X, 53HCONVERSION FROM THE
8 VERY NEAR FIELD TO THE NEAR FIELD/15X, 9HMODEL (M)//)
272 FORMAT(4X,
171HTRD(I,5) = THE CONVERSION POINT FROM THE NEAR FIELD TO
2 THE INTERMEDIATE/15X, 37HFIELD IN THE STREAMWISE DIRECTION (M)
3//4X, 52HTRD(I,6) = THE AVERAGE CONCENTRATION AT THE POINT OF
4/15X, 37HCONVERSION FROM THE NEAR FIELD TO THE/15X, 28HINTERMEDIATE
5 FIELD (KG/M**3)//4X, 60HTRD(I,7) = THE ADJUSTMENT IN THE X
6 DIRECTION AT THE POINT OF/15X, 56HCONVERSION FROM THE NEAR FIELD
7 TO THE INTERMEDIATE FIELD/15X, 9HMODEL (X)//X, 76H TRD(I,1)
8 TRD(I,2) TRD(I,3) TRD(I,4) TRD(I,5) TRD(I,6)
9 TRD(I,7)//)
271 FORMAT(7(X,E10.3)//)
1000 RETURN
END
```

SUBROUTINE INSTAN

INPUT VARIABLES:

H = INTEGRATION STEP SIZE, M
K1 = PARAMETER TO ALLOW DEFAULT VALUE OF H TO BE USED.
K1=1 REQUIRES USER INPUT. K1=2 USES DEFAULT VALUE
AND USER INPUT IS NOT NEEDED
RHO = WATER DENSITY, KG/M**3
DENS = CHEMICAL SPILL DENSITY, KG/M**3
ACCLASS(J) = FLOW REGIME DESCRIPTION
TESTNO = EXPERIMENTAL TEST NUMBER
TPER = TIDAL PERIOD, S
WC = WIDTH OF THE CHANNEL, M
DC = DEPTH OF THE CHANNEL, M
AI_DC = DISTANCE IN THE Y DIRECTION FROM THE CHANNEL CENTERLINE TO
THE SPILL ORIGIN, M
BLOC = VERTICAL DISTANCE DOWN FROM THE WATER SURFACE TO
THE SPILL ORIGIN, M
EYCOEF = Y DIFFUSION COEFFICIENT FOR THE NEAR FIELD MODEL
EZCOEF = Z DIFFUSION COEFFICIENT FOR THE NEAR FIELD MODEL
VNUM = RIVER FRICTION COEFFICIENT FOR FRICTION VELOCITY
K2 = PARAMETER TO ALLOW DEFAULT VALUES FOR EYCOEF, EZCOEF,
AND VNUM TO BE USED. K2=1 ALLOWS USER INPUT.
K2=2 USES DEFAULT VALUES AND USER INPUT IS NOT NEEDED
U1NF = MEAN RIVER VELOCITY, M/S
U2NF = MAXIMUM FLUCTUATING VELOCITY OF A TIDAL RIVER, M/S
ALFANF = PHASE SHIFT ANGLE FOR THE TIDAL RIVER PERIOD, SECONDS
HEVAP = EVAPORATION MASS TRANSFER COEFFICIENT, M/S
NOBS = NUMBER OF SETS OF X, Y, AND Z (NUMBER OF OBSERVATION POINTS)
XOB = DOWNSTREAM DISTANCE FROM THE LOCATION OF THE INSTANTANEOUS
SPILL TO THE OBSERVATION POINT, M
YOB = DISTANCE FROM THE CENTER OF THE CHANNEL TO THE OBSERVATION
POINT IN THE TRANSVERSE DIRECTION, M
ZOB = DISTANCE FROM THE CHANNEL SURFACE TO THE OBSERVATION
POINT IN THE VERTICAL DIRECTION, M
TLOW = STARTING OBSERVATION TIME, S
TDELT = TIME STEP, S
NSTEP = NUMBER OF DATA POINTS FOR EACH TIME STEP
SMASS = TOTAL MASS SPILLED, KG

DIMENSIONS:

```

DOUBLE PRECISION ACLASY(4), TESTNO(1)
INTEGER*4 NSTEP
REAL MEVAP
DIMENSION XOB(30), YOB(30), ZOB(30), TLOW(30), TDELT(30), NSTEP(30),
*VN(3), YVN(3)
DIMENSION PS(5, 5), XLS(5)
COMMON /ACT/EXCO, EYCO, EZCO, EEX, UEX, PI, ALOC, BLOC, DC,
1WC, SMASS, HEVAP, DENS, ROA, EXAVE, UEXAVE, UFS, H, NN
COMMON /ELSI/U1NF, U2NF, TPER, ALFANF, TLV, BETA, AKT, UPRI, RH, TMVN,
$IDE, RVNF, MEVAP
OPEN(UNIT=2, NAME='SYO: INSTIN. DAT', 0, READONLY, TYPE='OLD')
DATA PI/3. 1415927/
OC=9. 80665
DK=0. 0

```

READ IN PARAMETERS AND INITIAL CONDITIONS.

```

READ(2, 430) K1
READ(2, 418) WC, DC
H=0. 1+DC
IF (K1, EQ, 2) GO TO 6000
READ(2, 400) H
6000 READ(2, 401) ROA, DENS
READ(2, 411) (ACCLASS(J), J=1, 4)
READ(2, 415) TESTNO(1)
READ(2, 420) ALOC, BLOC
READ(2, 430) K2
EYCOEF=0. 6
EZCOEF=0. 067
VNUM=0. 025
IF (K2, EQ, 2) GO TO 6001
READ(2, 421) EYCOEF, EZCOEF, VNUM
6001 READ(2, 422) U1NF, U2NF, ALFANF, TPER
READ(2, 425) NOBS
DO 426 INT=1, NOBS
READ(2, 427) XOB(INT), YOB(INT), ZOB(INT)
READ(2, 428) TLOW(INT), TDELT(INT), NSTEP(INT)
426 CONTINUE
READ(2, 429) SMASS, HEVAP
C
C      PRINT PARAMETERS, HEADINGS AND INITIAL CONDITIONS.
C
      WRITE(3, 517)
      WRITE(3, 508) TESTNO(1)
      WRITE(3, 509) (ACCLASS(J), J=1, 4)
      WRITE(3, 535) ROA, DENS
      WRITE(3, 505) WC, DC
      WRITE(3, 506) ALOC, BLOC
      WRITE(3, 512) U1NF, U2NF, ALFANF, TPER
      WRITE(3, 564) SMASS, HEVAP, VNUM
      WRITE(3, 535) EYCOEF, EZCOEF
      WRITE(3, 514) H
      WRITE(3, 560) NOBS
      WRITE(3, 561)
      DO 562 INT=1, NOBS
      WRITE(3, 563) XOB(INT), YOB(INT), ZOB(INT), TLOW(INT), TDELT(INT),
      NSTEP(INT)
562 CONTINUE
C
C      FORMAT STATEMENTS FOR INPUT AND OUTPUT STATEMENTS.
C
400 FORMAT(2X, F10. 6)
401 FORMAT(4X, F9. 3, 7X, F9. 3)
411 FORMAT(4AB)
415 FORMAT(7X, A8)
418 FORMAT(3X, F9. 3, 5X, F9. 3)
420 FORMAT(9X, F10. 3, 7X, F10. 3)
421 FORMAT(7X, F10. 5, 9X, F10. 5, 7X, F10. 5)
422 FORMAT(5X, F8. 3, 7X, F8. 2, 9X, F8. 2, 7X, F10. 1)
425 FORMAT(5X, I3/)
427 FORMAT(4X, F12. 4, 2(6X, F12. 4))
428 FORMAT(5X, F10. 2, 8X, F10. 2, 8X, I6)
429 FORMAT(6X, F10. 4, 8X, F10. 4)
430 FORMAT(3X, I2)
505 FORMAT(6X, 21HO WIDTH OF CHANNEL = , F9. 3, 2H M)
1/6X, 21HO DEPTH OF CHANNEL = , F9. 3, 2H M)
506 FORMAT(6X, 80HO DISTANCE FROM THE CHANNEL CENTERLINE TO THE SPILL O
1RIGIN IN THE Y DIRECTION = , F10. 3, 2H M
2/6X, 80HO DISTANCE DOWN FROM THE WATER SURFACE TO THE SPILL
3 ORIGIN IN THE Z DIRECTION = , F10. 3, 2H M)

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508 FORMAT(2X, 10HTEST NO. :AB)
509 FORMAT(/2X, 24HFLOW FIELD DESCRIPTION: ,4AB/)
512 FORMAT(6X, 31H0 MEAN VELOCITY OF THE RIVER = ,F9. 3, 4H M/S/6X,
152H0 MAXIMUM FLUCTUATION VELOCITY OF THE TIDAL RIVER = ,F9. 3, 4H
2 M/S/6X, 36H0 PHASE SHIFT OF THE TIDAL PERIOD = ,F10. 4, 8H SECONDS
3/6X, 17H0 TIDAL PERIOD = ,F14. 4, 8H SECONDS)
514 FORMAT(6X, 36H0 NUMERICAL INTEGRATION STEP SIZE = ,F10. 6,
1 8H SECONDS)
517 FORMAT(1H1, /2X, 25HINSTANTANEOUS SPILL MODEL/)
526 FORMAT(1H1, 2X, 76HCONCENTRATION MATCHING DATA FOR POINTS OF
1 CONVERSION FOR THE VARIOUS MODELS:/)
527 FORMAT(/4X, 33HTURBULENT DIFFUSION COEFFICIENTS://7X,
1 11H0 EXCO = ,E11. 4/7X, 11H0 EYCO = ,E11. 4/7X,
2 11H0 EZCO = ,E11. 4)
535 FORMAT(/4X, 46HDIFFUSION FACTORS FOR THE NEAR FIELD EQUATION:/
1/7X, 21H0 EY COEFFICIENT = ,F10. 5/7X, 21H0 EZ COEFFICIENT = ,F10
2. 5//)
536 FORMAT(6X, 18H0 WATER DENSITY = ,F9. 3, 8H KG/M**3/6X,
127H0 CHEMICAL SPILL DENSITY = ,F9. 3, 8H KG/M**3)
560 FORMAT(6X, 64H0 NUMBER OF SETS OF X, Y, AND Z (NUMBER OF
1 OBSERVATION POINTS) = ,I3)
561 FORMAT(/6X, 51HOBSERVATION INFORMATION FOR AN INSTANTANEOUS
1 SPILL: //8X, 1HX, 13X, 1HY, 13X, 1HZ, 9X, 9HINIT TIME, 4X,
28HTIME INC, 3X, 13HNUMBER OF INC/5X, 8H(METERS), 6X, 8H(METERS),
36X, 8H(METERS), 6X, 9H(SECONDS), 3X, 9H(SECONDS)/)
563 FORMAT(3X, F12. 4, 2(2X, F12. 4), 3X, F10. 2, 2X, F10. 2, 2X, I6)
564 FORMAT(6X, 50H0 TOTAL SPILLED MASS FOR AN INSTANTANEOUS SPILL
1 = ,F10. 4, 3H KG/6X, 42H0 EVAPORATION MASS TRANSFER COEFFICIENT
2 = ,F10. 4, 4H M/S/6X, 29H0 CHANNEL ROUGHNESS FACTOR = ,F10. 5)

```

C
C
C

CALCULATE CONSTANTS

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RH=DC*WC/(2. 0*DC+WC)
UFS1=ABS(U1NF+SIN(2. 0*PI*ALFANF/TPER))
UFS2=(U1NF<<2+U2NF<<2)<<0. 5
IF (UFS1. GT. UFS2) UFS=UFS1
IF (UFS1. LE. UFS2) UFS=UFS2
UPRI=3. 807*VNUM*UFS/(RH**0. 16666667)
EXCOEF=EYCOEF*10.
EXCO=EXCOEF*DC*UPRI
EYCO=EYCOEF*DC*UPRI
EZCO=EZCOEF*DC*UPRI
WRITE(3, 527) EXCO, EYCO, EZCO
WRITE(3, 526)
EEX=5. 93*DC*UPRI
UEFX=0. 18*((UPRI*UFS)**0. 5)*WC**2/RH
FACT1=EZCO*TPER/DC**2
FACT2=PI**2/4.
FACT3=1. +FACT1/(2. *SQRT(FACT2+FACT1**2))
FACT4=SQRT(UFS*UPRI)*WC**2/RH
BETA=-ASIN(1./SQRT(FACT2*FACT1**2+1. ))
AKT=FACT1/SQRT(FACT2+FACT1**2)
EXAVE=5. 93*DC*UPRI*FACT3
UEXAVE=0. 18*FACT4*FACT3
MEVAP=0. 0
RVNF=0. 0
VNHO=(5MASS/(2. 0*PI*DENS))<<(1. 0/3. 0)
VNHO=2. 0*VNHO
SPVEL=1. 30*((QC*VNHO*ABS(1. 0-ROA/DENS))**0. 5)
IF(VNHO. LT. DC. AND. (3. 7*UPRI). LT. SPVEL)QO TO 120
IF(VNHO. LT. DC)QO TO 115
VNHO=DC
VNHO=(5MASS/(PI*DENS*DC))<<0. 5

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IF(VNRO.LT. (WC/4.0))GO TO 101
WRITE(3,580)
580 FORMAT(//6X,3BHSPILL IS TOO LARGE TO BE INSTANTANEOUS)
GO TO 2000
101 SPVEL=1.30*((GC*DC*ABS(1.0-ROA/DENS))**0.5)
IF((3.7*UPRI).LT.SPVEL)GO TO 120
C
C ***** ****
C
C NEUTRAL BUOYANCY CASE
115 IF(DENS.GT.ROA)GO TO 117
BLOC = 0.0
GO TO 118
117 BLOC=DC
118 CCPRI=DENS
TMVNF=0.0
ICASE=2
GO TO 21
C
C ***** ****
C
C STANDARD CASE
120 IF(DENS.GT.ROA)GO TO 124
TVNF=(2.0*BLOC/(GC*(ROA/DENS-1.0)))**0.5
BLOC=0.0
GO TO 130
124 TVNF=(2.0*(DC-BLOC)/(GC*(1.0-ROA/DENS)))**0.5
BLOC=DC
130 VNPRT=0.0
TTVNF=TVNF
CCPRI = VNEAR(0.0,0.0,0.0,0.0,0.0,TVNF,VNRO,GC,0.0,VNPRT)
ICASE=1
21 CONTINUE
C
C ***** ****
C
C WRITE(3,5548)CCPRI
5548 FORMAT(4X,3HVERY NEAR FIELD CONCENTRATION = ,1PE14.7,
1BH KG/M**3)
C
C COMPUTE MAXIMUM ALLOWABLE TIMES OF VARIOUS MODELS
C
22 TMAXNF=0.3*DC**2/EZCO
IF(TMAXNF.LT.(2.0*TMVNF))TMAXNF=2.0*TMVNF
TMAXIF=0.3*WC**2/EYCO
C
C COMPUTE FIRST GUESSES FOR MATCHING TIMES AND TIME INCREMENT
C
DDTO=.001*TMAXNF
DDT1=.002*TMAXNF
DNT2=.0005*TMAXIF
DTO=.1
DT1=.1
DT2=.1
C
C COMPUTE LOCATIONS OF POINT AND LINE SOURCES
C
DO 23 I=1,5
DO 23 J=1,5
C
C POINT SOURCE AT SPILL ORIGIN AND IMAGES
C
23 PS(I,J)=0.0

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```

PS(1, 1)=ALOC
PS(3, 1)=ALOC
PS(5, 1)=ALOC
PS(2, 1)=WC-ALOC
PS(4, 1)=-WC-ALOC
IF(ICASE.EQ.2)GO TO 160
C
C      POINT SOURCES TO ACCOUNT FOR GRAVITY SPREADING
C      FIRST, ASSUME SPILL DOES NOT HIT EITHER WALL
C
DO 140 I=1,4
J=I+1
IF(J.LT.4)AVNF=1
IF(J.GE.4)AVNF=-1
PS(1, J)=PS(1, 1)+I*AVNF*RVNF/3. 0
PS(3, J)=PS(1, J)
PS(5, J)=PS(1, J)
PS(2, J)=PS(2, 1)-I*AVNF*RVNF/3. 0
PS(4, J)=PS(4, 1)-I*AVNF*RVNF/3. 0
140 CONTINUE
IF(IDEC.EQ.1)GO TO 160
C
C      NOW, CORRECT FOR SPILL HITTING CLOSEST WALL
C
PS(1, 2)=2. *ALOC/3. +WC/6.
PS(2, 2)=5. *WC/6. -2. *ALOC/3.
PS(4, 2)=-7. *WC/6. -2. *ALOC/3.
PS(1, 3)=WC/3. +ALOC/3.
PS(2, 3)=2. *WC/3. -ALOC/3.
PS(4, 3)=-4. *WC/3. -ALOC/3.
DO 153 N=2,5
PS(3, N)=PS(1, N)
153 PS(5, N)=PS(1, N)
IF(IDEC.EQ.2)GO TO 160
C
C      NOW, CORRECT FOR SPILL HITTING BOTH WALLS
C
PS(1, 4)=2. *ALOC/3. -WC/6.
PS(2, 4)=7. *WC/6. -2. *ALOC/3.
PS(4, 4)=-5. *WC/6. -2. *ALOC/3.
PS(1, 5)=ALOC/3 -WC/3.
PS(2, 5)=1. *WC/3. -ALOC/3.
PS(4, 5)=-2. *WC/3 -ALOC/3.
DO 157 N=2,5
PS(3, N)=PS(1, N)
157 PS(5, N)=PS(1, N)
160 CONTINUE
DO 170 N=1,5
XLS(N)=PS(1, N)
170 CONTINUE
C
C      MATCH NEAR FIELD TO VERY NEAR FIELD MODEL
C
TT=0. 0
XX=0. 0
YCPRI=ALOC
ZCPRI=BLOC
336 CONV=RNEAR(XX, YCPRI, ZCPRI, TT, DTO, PS, ICASE)
DCON=CONV/CCPRI
DCON=ABS(1. -DCON)
IF(DCON.LE.0. 001)GO TO 330
IF(DCON.LE.0. 01)GO TO 338
IF(DCON.LE.0. 1)GO TO 339

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340 DTO=DTO+DDTO
  CONV=RNEAR(XX, YCPRI, ZCPRI, TT, DTO, PS, ICASE)
  DCON=CONV/CCPRI
  DCON=ABS(1. -DCON)
  IF(DCON. LE. 0. 001)GO TO 330
  IF(DCON. LE. 0. 01)GO TO 338
  IF(DCON. LE. 0. 1)GO TO 339
  GO TO 340
339 DTO=DTO-DDTO
  DDTO=DDTO/10.
341 DTO=DTO+DDTO
  CONV=RNEAR(XX, YCPRI, ZCPRI, TT, DTO, PS, ICASE)
  DCON=CONV/CCPRI
  DCON=ABS(1. -DCON)
  IF(DCON. LE. 0. 001)GO TO 330
  IF(DCON. LE. 0. 01)GO TO 338
  GO TO 341
338 DTO=DTO-DDTO
  DDTO=DDTO/10.
342 DTO=DTO+DDTO
  CONV=RNEAR(XX, YCPRI, ZCPRI, TT, DTO, PS, ICASE)
  DCON=CONV/CCPRI
  DCON=ABS(1. -DCON)
  IF(DCON. LE. 0. 001)GO TO 330
  GO TO 342
330 WRITE(3, 5547)CONV
  DTO=DTO-TMAXNF
5547 FORMAT(/4X, 27HNEAR FIELD CONCENTRATION = , 1PE14. 7, 8H KG/M**3)
C
C      MATCH INTERMEDIATE FIELD MODEL TO NEAR FIELD MODEL
C
  VELD=VEL OC(TMAXNF)
  COND=AVENF(TMAXNF, VELD, ALOC, BLOC, VELD, PS, ICASE)
  WRITE(3, 5550)COND
5550 FORMAT(/4X, 35HAVERAGE NEAR FIELD CONCENTRATION = , 1PE14. 8,
18H KG/M**3)
  CONDI=RMEIDI(VELD, ALOC, BLOC, TMAXNF, DT1, XLS, ICASE)
  DCON=COND/COND
  DCON=ABS(1. -DCON)
  IF(DCON. LE. 0. 001)GO TO 250
  IF(DCON. LE. 0. 01)GO TO 240
  IF(DCON. LE. 0. 1)GO TO 230
231 DT1=DT1+DDT1
  CONDI=RMFDI(VELD, ALOC, BLOC, TMAXNF, DT1, XLS, ICASE)
  DCON=COND/COND
  DCON=ABS(1. -DCON)
  IF(DCON. LE. 0. 001)GO TO 250
  IF(DCON. LE. 0. 01)GO TO 240
  IF(DCON. LE. 0. 1)GO TO 230
  GO TO 231
230 DT1=DT1-DDT1
  DDT1=DDT1/10.
241 DT1=DT1+DDT1
  CONDI=RMFDI(VELD, ALOC, BLOC, TMAXNF, DT1, XLS, ICASE)
  DCON=COND/COND
  DCON=ABS(1. -DCON)
  IF(DCON. LE. 0. 001)GO TO 250
  IF(DCON. LE. 0. 01)GO TO 240
  GO TO 241
240 DT1=DT1-DDT1
  DDT1=DDT1/10.
242 DT1=DT1+DDT1
  CONDI=RMFDI(VELD, ALOC, BLOC, TMAXNF, DT1, XLS, ICASE)

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DCON=COND1/COND0
DCON=ABS(1. -DCON)
IF(DCON. LE. 0. 001)GO TO 250
GO TO 242
250 WRITE(3, 5549)COND1
5549 FORMAT(/4X, 35HINTERMEDIATE FIELD CONCENTRATION = , 1PE14. 8,
18H KG/M**3)
VVELD=VELOC(TMAXIF)
DT11=0. 0
COND=AVEIF(TMAXIF, VVELD, DT11)
WRITE(3, 5552)COND
5552 FORMAT(/4X, 43HAVERAGE INTERMEDIATE FIELD CONCENTRATION = ,
11PE14. 8, 8H KG/M**3)

C
C      MATCH FAR FIELD MODEL TO INTERMEDIATE FIELD MODEL
C
CONF=FAR(VVELD, ALOC, BLOC, TMAXIF, DT2)
DCON=CONF/COND
DCON=ABS(1. -DCON)
IF(DCON. LE. 0. 001)GO TO 293
IF(DCON. LE. 0. 01)GO TO 233
IF(DCON. LE. 0. 05)GO TO 253
IF(DCON. LE. 0. 2)GO TO 252
244 D12=DT2+DDT2
CONF=FAR(VVELD, ALOC, BLOC, TMAXIF, DT2)
DCON=CONF/COND
DCON=ABS(1. -DCON)
IF(DCON. LE. 0. 001)GO TO 293
IF(DCON. LE. 0. 01)GO TO 233
IF(DCON. LE. 0. 05)GO TO 253
IF(DCON. LE. 0. 2)GO TO 252
GO TO 244
252 D12=DT2-DDT2
DDT2=DDT2/10.
247 D12=DT2+DDT2
CONF=FAR(VVELD, ALOC, BLOC, TMAXIF, DT2)
DCON=CONF/COND
DCON=ABS(1. -DCON)
IF(DCON. LE. 0. 001)GO TO 293
IF(DCON. LE. 0. 01)GO TO 233
IF(DCON. LE. 0. 05)GO TO 253
GO TO 247
253 DT2=DT2-DDT2
DDT2=DDT2/10.
248 DT2=DT2+DDT2
CONF=FAR(VVELD, ALOC, BLOC, TMAXIF, DT2)
DCON=CONF/COND
DCON=ABS(1. -DCON)
IF(DCON. LE. 0. 001)GO TO 293
IF(DCON. LE. 0. 01)GO TO 233
GO TO 248
233 DT2=DT2-DDT2
DDT2=DDT2/10.
290 D12=DT2+DDT2
CONF=FAR(VVELD, ALOC, BLOC, TMAXIF, DT2)
DCON=CONF/COND
DCON=ABS(1. -DCON)
IF(DCON. LE. 0. 001)GO TO 293
GO TO 290
293 WRITE(3, 5554)CONF
5554 FORMAT(/4X, 26HFAR FIELD CONCENTRATION = , 1PE14. 8, 8H KG/M**3)
WRITE(3, 5599)TMVN, TMAXNF, TMAXIF
5599 FORMAT(///3X, 40HCONVERSION TIMES FOR THE VARIOUS MODELS: //)

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14X, 31HMAXIMUM VERY NEAR FIELD TIME = , 1PE13. 7, 4H SEC/
2/4X, 26HMAXIMUM NEAR FIELD TIME = , 1PE13. 7, 4H SEC//4X,
334HMAXIMUM INTERMEDIATE FIELD TIME = , 1PE13. 7, 4H SEC///)
WRITE(3, 302) DTO, DT1, DT2

302 FORMAT(3X, 40HCORRECTION TIMES FOR THE VARIOUS MODELS: //4X,
129HNEAR FIFLD CORRECTION TIME = , 0PF12. 4, 4H SEC//4X,
237HINTERMEDIATE FIELD CORRECTION TIME = , 0PF12. 4, 4H SEC//4X,
328HFAR FIELD CORRECTION TIME = , 0PF12. 4, 4H SEC)

C
C      CALCULATION LOOP FOR EACH OBSERVATION POINT
C

DO 1000 III=1, NOBS
TIME=TLow(III)
WRITE(3, 303) XOB(III), YOB(III), ZOB(III)

300 FORMAT(1H1, 2X, 37HCOORDINATES OF THE OBSERVATION POINT: ///
14X, 22HDOWNSTREAM DISTANCE = , 0PF10. 4, 2H M//4X, 50HTRANSVERSE
2 DISTANCE FROM THE CHANNEL CENTERLINE = , 0PF10. 4, 2H M//4X,
343HVERTICAL DISTANCE FROM THE WATER SURFACE = , 0PF10. 4, 2H M
4///)
WRITE(3, 305)

305 FORMAT(6X, 4HTIME, 8X, 13HCONCENTRATION, 8X, 21HTOTAL MASS EVAPORATED/
$4X, 9H(SECONDS), 7X, 9H(KG/M**3), 18X, 4H(KG)/)

C      DETERMINE IF VERY NEAR FIELD IS NEEDED
NN=0
IF(TIME.GT. TMVNF)GO TO 10
ANN=(TMVNF-TIMF)/TDELT(III)
NN=ANN+1
IF(NN.GT. NSTEP(III))NN=NSTEP(III)

C      CALCULATE VERY NEAR FIELD CONCENTRATION
PRINTING IS DONE IN VNEAR ITSELF
VNPR=1.
TD=TDELT(III)
PRTM=TIME
CON=VNEAR(XOB(III), YOB(III), ZOB(III), PRTM, TTVNF, VNRO, GC, TD, VNPR)
IF(NN.EQ. NSTEP(III))GO TO 1000
TIME=TIME+NN*TD

C
C      IF NONE OF THE OBSERVATION TIME IS IN THE VERY NEAR FIELD
C      OR IF ONLY PART OF THE TOTAL OBSERVATION TIME PERIOD IS IN
C      THE VERY NEAR FIELD, THE OTHER FIELDS MUST BE USED
C

10 NNN=NN+1
DO 1001 JJJ=NNN, NSTEP(III)
IF(TIME.LT. (TMAXNF-DTO))GO TO 11
IF(TIME.LT. (TMAXIF-DTO-DT1))GO TO 12
GO TO 13
C      CALCULATE NEAR FIELD CONCENTRATION
11 CON=RNEAR(XOB(III), YOB(III), ZOB(III), TIME, DTO, PS, ICASE)
GO TO 100
C      CALCULATE INTERMEDIATE FIELD CONCENTRATION
12 DT11=DT1-DTO
CON=RMEDI(XOB(III), YOB(III), ZOB(III), TIME, DT11, XLS, ICASE)
GO TO 100

C
C      CALCULATE FAR FIELD CONCENTRATION
C

13 DT22=DT2+DT1-DTO
CON=FAR(XOB(III), YOB(III), ZOB(III), TIME, DT22)
100 WRITE(3, 303) TIME, CON, MEVAP
303 FORMAT(3X, F10. 2, 4X, 1PE19. 8, 7X, E19. 8)
TIME=TIME+TDELT(III)

1001 CONTINUE
1000 CONTINUE

```

```

      RETURN
2000 END
C
      FUNCTION AVENF(T, X, Y, Z, U, PS, ICASE)
      REAL MEVAP
      DIMENSION PS(3, 5)
      COMMON /ACT/EXCO, EYCO, EZCO, EEX, UEXX, PI, ALOC, BLOC, DC,
      1WC, SMASS, HFVAP, DENS, ROA, EXAVE, UEXAVE, UFS, H, NN
      COMMON /ELSI/U1NF, U2NF, TPER, ALFANF, TLV, BETA, AKT, UPRI, RH, TMVNF,
      *IDEC, RVNF, MEVAP
      DK=0.0

C
C      THIS FUNCTION CALCULATES AVERAGE NEAR FIELD CONCENTRATION
C

      IF(ICASE.EQ.1)N=5
      IF(ICASE.EQ.2)N=1
      IF(ICASE.EQ.1)SMAS=(SMASS-MEVAP)/5.
      IF(ICASE.EQ.2)SMAS=SMASS
      CONN1=SMAS*EXP(-DX*T)/((4.*PI*T)**1.5)
      CONN2=CONN1*EXP(-(X-U)**2. / (4.*EXCO*T))
      CONN3=CONN2/((EXCO*EYCO*EZCO)**0.5)
      CONN3=CONN3*((PI*EZCO*T/(DC**2. ))**0.5)
      CON1=0.
      CON2=0.
      CON3=0.
      CON4=0.
      CON5=0.
      D1=(DC-BL_DC)/((4.*EZCO*T)**0.5)
      D2=D1
      D3=(DC-2.*DC+BLOC)/((4.*EZCO*T)**0.5)
      D4=D1
      D5=(DC+BLOC)/((4.*EZCO*T)**0.5)
      E1=BLOC/((4.*EZCO*T)**0.5)
      E2=E1
      E3=(2.*DC-BLOC)/((4.*EZCO*T)**0.5)
      E4=E1
      E5=(-BLOC)/((4.*EZCO*T)**0.5)
      DO 100 J=1,N
      CON1=CON1+EXP(-(Y-PS(1,J))**2. / (4.*EYCO*T))
      **(ERRF(D1)+ERRF(E1))
      CON2=CON2+EXP(-(Y-PS(2,J))**2. / (4.*EYCO*T))
      **(ERRF(D2)+ERRF(E2))
      CON3=CON3+EXP(-(Y-PS(3,J))**2. / (4.*EYCO*T))
      **(ERRF(D3)+ERRF(E3))
      CON4=CON4+EXP(-(Y-PS(4,J))**2. / (4.*EYCO*T))
      **(ERRF(D4)+ERRF(E4))
      CON5=CON5+EXP(-(Y-PS(5,J))**2. / (4.*EYCO*T))
      **(ERRF(D5)+ERRF(E5))
100  CONTINUE
      AVENF=CONN3*(CON1+CON2+CON3+CON4+CON5)
      RETURN
      END

C
      FUNCTION AVEIF(T, X, DT1)
      REAL MEVAP
      COMMON /ACT/EXCO, EYCO, EZCO, EEX, UEXX, PI, ALOC, BLOC, DC,
      1WC, SMASS, HFVAP, DENS, ROA, EXAVE, UEXAVE, UFS, H, NN
      COMMON /ELSI/U1NF, U2NF, TPER, ALFANF, TLV, BETA, AKT, UPRI, RH, TMVNF,
      *IDEC, RVNF, MEVAP
      DK=0.0

C
C      THIS FUNCTION CALCULATES AVERAGE INTERMEDIATE FIELD
C      CONCENTRATION AT THE BOUNDARY

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```

C
      SMAS=SMASS-MEVAP
      UT=VELOC(T)
      AREA=DC*WC
      CONM1=SMAS*EXP(-DX*(T-DT1))/((4.*PI*EEX*(T-DT1))**0.5*AREA)
      AVEIF=CONM1*EXP(-(X-UT)**2/(4.*EEX*(T-DT1)))
      RETURN
      END

C
      FUNCTION RNEAR(X, Y, Z, T, DTO, PS, ICASE)
      REAL MEVAP
      DIMENSION PS(5, 5)
      COMMON /ACT/EXCO, EYCO, EZCO, EEX, UEXX, PI, ALOC, BLOC, DC,
      1WC, SMASS, H*VAP, DENS, ROA, EXAVE, UEXAVE, UFS, H, NN
      COMMON /ELSI/U1NF, U2NF, TPER, ALFANF, TLV, BETA, AKT, UPRI, RH, TMVNF,
      *IDEC, RVNF, MEVAP
      DK=0.0

C
C      THIS FUNCTION CALCULATES NEAR FIELD CONCENTRATION
C
      DBX=4.*EXCO*(T+DTO)
      DBY=4.*EYCO*(T+DTO)
      DBZ=4.*EZCO*(T+DTO)
      U=VELOC(T)
      IF(ICASE.EQ.1)N=5
      IF(ICASE.EQ.2)N=1
      IF(ICASE.EQ.1)SMAS=(SMASS-MEVAP)/5.
      IF(ICASE.EQ.2)SMAS=SMASS
      CONO=SMAS*EXP(-DX*(T+DTO)-(X-U)**2./DBX)
      CONO=CONO/((4.*PI*(T+DTO))**1.5*(EXCO*EYCO*EZCO)**0.5)
      CON1=0.
      CON2=0.
      CON3=0.
      CON4=0.
      CON5=0.
      DO 100 J=1,N
      CON1=CON1+EXP(-((Y-PS(1,J))**2./DBY-(Z-BLOC)**2./DBZ)
      CON2=CON2+EXP(-((Y-PS(2,J))**2./DBY-(Z-BLOC)**2./DBZ)
      CON3=CON3+EXP(-((Y-PS(3,J))**2./DBY-(Z-2.*DC+BLOC)**2./DBZ)
      CON4=CON4+EXP(-((Y-PS(4,J))**2./DBY-(Z-BLOC)**2./DBZ)
      CON5=CON5+EXP(-((Y-PS(5,J))**2./DBY-(Z+BLOC)**2./DBZ)
100  CONTINUE
      RNEAR=CONO+(CON1+CON2+CON3+CON4+CON5)
      RETURN
      END

C
      FUNCTION RMEDI(X, Y, Z, T, DT1, XLS, ICASE)
      REAL MEVAP
      DIMENSION XLS(5)
      COMMON /ACT/EXCO, EYCO, EZCO, EEX, UEXX, PI, ALOC, BLOC, DC,
      1WC, SMASS, H*VAP, DENS, ROA, EXAVE, UEXAVE, UFS, H, NN
      COMMON /ELSI/U1NF, U2NF, TPER, ALFANF, TLV, BETA, AKT, UPRI, RH, TMVNF,
      *IDEC, RVNF, MEVAP
      DK=0.0

C
C      THIS FUNCTION CALCULATES INTERMEDIATE FIELD CONCENTRATION
C
      IF(ICASE.EQ.1)NN=5
      IF(ICASE.EQ.2)NN=1
      IF(ICASE.EQ.1)SMAS=(SMASS-MEVAP)/5.
      IF(ICASE.EQ.2)SMAS=SMASS
      AREA=WC*DC
      UT=VELOC(T)

```

```

IF(U2NF. NE. 0. )EEX=EXAVE
CONO=SMAS/((4. *PI*EEX*(T-DT1))**0. 5*AREA)
CONO=CONO*EXP(-DK*(T-DT1)-(X-UT)**2/(4. *EEX*(T-DT1)))
CON1=0
DO 200 M=1,NN
DO 100 N=1,20
AN=N
CON2=COS(AN*PI*(WC/2.+XLS(M))/WC)*COS(AN*PI*(WC/2.+Y)/WC)
CON2=CON2*EXP(-AN**2.*PI**2.*EYCO*(T-DT1)/(WC**2.))
CON1=CON1*CON2
100 CONTINUE
200 CONTINUE
RMEDI=CONO*(1.+2.*CON1)
IF(U2NF. EQ. 0. )GO TO 221
EXT=1. 483*DC*UPRI*FACT(T)
RMEDI=RMEDI*(1.+EXT/EEX*(X-UT)**2. /(4.*EEX*(T-DT1)))
IF (RMEDI.LT. 0. 0) RMEDI=0. 0
221 RETURN
END
C
FUNCTION FAR(X, Y, Z, T, DT2)
REAL MEVAP
COMMON /ACT/EXCO, EYCO, EZCO, EEX, UEXX, PI, ALOC, BLOC, DC,
WC, SMAS, H-VAP, DENS, ROA, EXAVE, UEXAVE, UFS, H, NN
COMMON /ELSI/U1NF, U2NF, TPER, ALFANF, TLV, BETA, AKT, UPRI, RH, TMVNF,
*IDEC, RVNF, MEVAP
DK=0. 0
C
C THIS FUNCTION CALCULATES FAR FIELD CONCENTRATION
C
SMAS=SMASS-MEVAP
AREA=WC*DC
UT=VELOC(T)
IF(U2NF. NE. 0. )UEEX=UEXAVE
CONO=SMAS/(AREA*(4.*PI*UEEX*(T-DT2))**0. 5)
FAR=CONO*EXP(-DK*(T-DT2)-(X-UT)**2/(4.*UEEX*(T-DT2)))
IF(U2NF. EQ. 0. )GO TO 122
UEXT=(0. 045*SQRT(UFS*UPRI)*WC**2/RH)*FACT(T)
FAR=FAR*(1.+((X-UT)**2/(4.*UEEX*(T-DT2)))*UEXT/UEEX)
IF (FAR.LT. 0. 0) FAR=0. 0
122 RETURN
END
C
FUNCTION VELOC(T)
REAL MEVAP
COMMON /ACT/EXCO, EYCO, EZCO, EEX, UEXX, PI, ALOC, BLOC, DC,
WC, SMAS, H-VAP, DENS, ROA, EXAVE, UEXAVE, UFS, H, NN
COMMON /ELSI/U1NF, U2NF, TPER, ALFANF, TLV, BETA, AKT, UPRI, RH, TMVNF,
*IDEC, RVNF, MEVAP
DK=0. 0
C
C THIS FUNCTION CALCULATES THE INTEGRAL OF THE CHANNEL VELOCITY
C W. R. T. TIME
C
VEL1=COS(2.*PI/TPER*(T+ALFANF))-COS(2.*PI*ALFANF/TPER)
VELOC=U1NF+T-U2NF+TPER/(2.*PI)*VEL1
RETURN
END
C
FUNCTION ERRF(XX)
X=XX
IF(XX. LT. 0. )X=-XX
A1=0. 34802

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```

A2=-0.09587
A3=0.74785
A4=0.47047
YY=1./(1.+A4*X)
ERRF=1.-(A1*YY+A2*YY**2+A3*YY**3)*EXP(-X**2)
IF(XX.LT.0.)ERRF=-ERRF
RETURN
END
C
C      FUNCTION FACT(T)
C
C      REAL MEVAP
COMMON /ACT/EXCO,EYCO,EZCO,EEX,UEEX,PI,ALOC,BLOC,DC,
IWC,SMASS,HVAP,DENS,ROA,EXAVE,UEXAVE,UFS,H,NN
COMMON /ELSI/U1NF,U2NF,TPER,ALFANF,TLV,BE1A,AKT,UPRI,RH,TMVNF,
*IDEC,RVNF,MEVAP
DK=0.0
C
C      THIS FUNCTION CALCULATES THE TIDAL FACTOR
C
F1=AKT*SIN(2.0*PI/TPER*(T+ALFANF+BETA))+4.0*SIN(2.0*PI/TPER*(T+
ALFANF))
FACT=F1-AKT+COS(4.*PI/TPER*(T+ALFANF+0.5*BETA))
RETURN
END

```

```

FUNCTION VNPAR(X, Y, Z, T, TO, RI, QC, TD, VNPRT)
DIMENSION YVNF(3), VNF(3)
INTEGER RUNCE
REAL MEVAP
COMMON /ACT/EXCO, EYCO, EZCO, EEX, UEEX, PI, ALOC, BLOC, DC,
1WC, SMASS, HEVAP, DENS, ROA, EXAVE, UEXAVE, UFS, H, NN
COMMON /ELSI/U1NF, U2NF, TPER, ALFANF, TLV, BETA, AKT, UPRI, RH, TMVNF,
$IDECK, RVNF, MEVAP

C
C      THIS FUNCTION CALCULATES VERY NEAR FIELD CONCENTRATION
C
C      COMPUTE INITIAL RIGHT HAND SIDES
C      YVNF(1)=SPILL RADIUS
C      YVNF(2)=WATER MASS ENTRAINED
C      FRIC=USTAR COEFF=3.807*VNUM/(RH**1. /6. )
C      ICOUNT=1
C      MEVAP=0. 0
C      YVNF(1)=0.
C      YVNF(2)=0.
C      YVNF(3)=0.
C      RO-RI
C      FRIC=UPRI/UFS
C      TH0=SMASS/(PI*DENS*(RO**2. ))
C      VNF(1)=1. 3*((QC*TH0*ABS(1. 0-ROA/DENS))**0. 5)
C      VNFO=VNF(1)
C      UPRIS=MODIFIED FRICTION VELOCITY
C      UPRIS=FRIC*(((2.*VNF(1)/3)**2. +UFS**2. )**0. 5)
C      RINO=RICHARDSON NO.
C      RINO=0. 59*(VNF(1)**2. )/((1. 3*UPRIS)**2. )
C      U1UP=1. 3*UPRIS/(6. 00+0. 25*RINO)
C      USIDE=2. *(FRIC**2. )*VNF(1)
C      INITIAL DR/DT=DENOM OF USIDE DEFINITION
C      UE=UTOP+2. *(TH0/RO)*USIDE
C      VNF(2)=ROA*PI*UE*(RO**2. )
C      TVNF=TO
C      OLDMW=0. 0
C      OLDR0=0. 0
C      OLDM1E=0. 0
C      RO0=RO
C      ANC1=0. 0
C      ANC2=0. 0
C      TVNF=STARTING TIME OLDMW=INITIAL WATER ENTRAINMENT
C      OLDR0=STARTING RADIUS OLDM1E=INITIAL MASS EVAPORATED
C      IF(DENS. GT. ROA)GO TO 1
C      N=3
C      VNF(3)=PI*(RO**2. )*HEVAP*DENS
C      GO TO 2
1     N=2
      VNME=0. 0
C      VNME=TEMPORARY VALUE OF EVAPORATED MASS
C      IF(VNPRT. LT. 0. 5)GO TO 2
2     IRUNG=RUNGE(N, YVNF, VNF, TVNF, H)
C      IF(IRUNG. EQ. 0)GO TO 6
C      COMPUTE NEW RIGHT HAND SIDES
C      IF(N. EQ. 2)GO TO 3
      VNME=(OLDMW+YVNF(3))/2.
      OLDM1E=YVNF(3)
3     VNMW=(OLDMW+YVNF(2))/2.
      OLDMW=YVNF(2)
C      RHOM=MIXTURE DENSITY
      RHOM=(SMASS-VNME+VNMW)/((SMASS-VNME)/DENS+VNMW/ROA)
C      VNCON=SPILL CONCENTRATION

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VNCON=(SMASS-VNME)/((SMASS-VNME)/DENS+VNMF/ROA)
RO=(OLDRO+YVNF(1)+2.*RO0)/2.
OLDRO=YVNF(1)
C VNIHK=SPILL THICKNESS
VNTHK=((SMASS-VNME)/DENS+VNMF/ROA)/(PI+RO**2.)
C DETERMINE WHICH THICKNESS APPLIES
IF(RO.LE.(WC/2.-ALOC))GO TO 5
ANG1=2.*ASIN(1.-((WC/2.-ALOC)/RO)**2.)
IF(RO.GT.(WC/2.+ALOC))GO TO 4
VNTHK=VNTHK*(1.+0.5*(ANG1-SIN(ANG1))/PI)
GO TO 5
4 ANG2=2.*ASIN(1.-((WC/2.+ALOC)/RO)**2.)
VNTHK=VNTHK*(1.+0.5*(ANG1-SIN(ANG1))/PI+0.5*(ANG2
-$-SIN(ANG2))/PI)
5 VNF(1)=1.3*((QC*VNTHK*ABS(1.0-ROA/RHOM))**0.5)
UPRIS=FRIC*((2.*VNF(1)/3.)**2.+UFS**2.)*0.5
RINO=0.59*(VNF(1)**2.)/((1.3*UPRIS)**2.)
UTOP=1.3*UPRIS/(6.00+0.25*RINO)
USIDE=2.*((FRIC**2.)*(VNF(1)**2.)/VNFO
UE=UTOP+2.*((VNTHK/RO)*USIDE
VNF(2)=PI*ROA*(RO**2.)*UE*(1-0.5*(ANG1-SIN(ANG1))/PI
-$-0.5*(ANG2-SIN(ANG2))/PI)
IF(N.EQ.2)GO TO 2
VNF(3)=PI*(RO**2.)*HEVAP*VNCON*(1-0.5*(ANG1-SIN(ANG1))/PI
-$-0.5*(ANG2-SIN(ANG2))/PI)
GO TO 2
C COMPUTE VALUES AT END OF TIME STEP
6 IF(N.EQ.3)GO TO 7
VNME=0.0
GO TO 8
7 VNME=YVNF(3)
8 CCPRI=(SMASS-VNME)/((SMASS-VNME)/DENS+YVNF(2)/ROA)
RRO=YVNF(1)+RO0
ANG1=0.0
ANG2=0.0
VNTHK=((SMASS-VNME)/DENS+YVNF(2)/ROA)/(PI*(RRO**2.))
IF(YVNF(1).LE.(WC/2.-ALOC))GO TO 10
ANG1=2.*ASIN(1.-((WC/2.-ALOC)/(RRO**2.)))
IF(YVNF(1).GT.(WC/2.+ALOC))GO TO 9
GO TO 10
9 ANG2=2.*ASIN(1.-((WC/2.+ALOC)/(RRO**2.)))
VNTHK=VNTHK*(1.+0.5*(ANG1-SIN(ANG1))/PI+0.5*(ANG2-
-$-SIN(ANG2))/PI)
C DETERMINE IF GRAVITY SPREADING IS OVER
10 RHOM=(SMASS-VNME+YVNF(2))/((SMASS-VNME)/
$DENS+YVNF(2)/ROA)
VTEST=1.3*((QC*VNTHK*ABS(1.-ROA/RHOM))**0.5)
IF(VTEST.LE.(3.70*UPRI))GO TO 12
C PRINT OUTPUT IF VNPRT=1.0
IF(VNPRT.LT.0.5)GO TO 11
C CHECK IF INTEGRATION TIME IS PRINT-OUT TIME
IF(TVNF.LE.T)GO TO 11
VNEAR=CCPRI
C CHECK IF X,Y,Z IS IN SPILL
VNFX1=VELOC(T)+(YVNF(1)+RO0)
VNFX2=VELOC(T)-(YVNF(1)+RO0)
IF(X.OE.VNFX1)VNEAR=0.0
IF(X.LE.VNFX2)VNEAR=0.0
IF(Y.OE.(YVNF(1)+ALOC))VNEAR=0.0
IF(Y.LE.(-YVNF(1)+ALOC))VNEAR=0.0
IF(DENS.GT.ROA)GO TO 50
IF(Z.GT.VNIHK)VNEAR=0.0
GO TO 60

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50 IF(Z.LE.(DC-VNIHK))VNEAR=0.0
60 WRITE(3,103)T,VNEAR,YVNF(3)
ICOUNT=ICOUNT+1
C     INCREASE PRINT-OUT TIME BY TIME-STEP
T=T+TD
IF(ICOUNT.GT.NN)VNPRT=0.
IF(T.LT.THVNFT)GO TO 11
IF(N.EQ.2)MEVAP=YVNF(3)
RETURN
11 VNF(1)=VTEST
RRO=YVNF(1)+R00
UPRIS=FRIC*((2.*VNF(1)/3.)**2.+UFS**2.)***.5)
RINO=0.59*(VNF(1)**2.)/((1.3*UPRIS)**2.)
UTOP=1.3*UPRIS/(6.00+0.25*RINO)
USIDE=2.*FRIC**2.**(VNF(1)**2.)/VNFO
UE=UTOP+2.*(VN1HK/RRO)*USIDE
VNF(2)=PI*R0A*UE*(RRO**2.)*(1-0.5*(ANG1-SIN(ANG1))/PI
*-0.5*(ANG2-SIN(ANG2))/PI)
IF(N.EQ.2)GO TO 2
VNF(3)=PI*(RRO**2.)*HEVAP*CCPRI*(1-0.5*(ANG1-SIN(ANG1))/PI
*-0.5*(ANG2-SIN(ANG2))/PI)
GO TO 2
12 TMVNF=TVNF
RVNF=YVNF(1)+R00
IF(N.EQ.3)MVAP=YVNF(3)
IDEC=2
IF(RVNF.LE.(WC/2.-ALOC))IDEC=1
IF(RVNF.GT.(WC/2.+ALOC))IDEC=3
VNEAR=CCPRI
103 FORMAT(3X,F10.2,4X,1PE15.8,7X,E15.8)
100 RETURN
ENI)

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C *****PROGRAM STEADY*****
C
C PROJECT NO. : 02-5864-003
C PROJECT SPONSOR: COAST GUARD
C
C THIS PROGRAM CALCULATES THE PLUME TRAJECTORY AND PLUME CONCEN-
C TRATION OF A LIQUID CHEMICAL CONTINUOUSLY SPILLED INTO A BODY OF
C WATER HAVING A CONSTANT VELOCITY.
C
C INPUT FILE NAMES: SPILLIN.DAT
C OUTPUT FILE NAMES: SPILLOUT.DAT
C
C SUBROUTINE STEADY
C
C INPUT VARIABLES:
C
C      X = STARTING VALUE OF PLUME PATH INTEGRATION, M
C      H = INTEGRATION STEP SIZE, M
C      DISTA = INITIAL DOWNSTREAM DISTANCE TO THE FIRST PRINTOUT, M
C      DISTAN = INCREMENTAL DOWNSTREAM DISTANCE BETWEEN PRINTOUTS, M
C      ROA = AMBIENT FLUID DENSITY, KG/M**3
C      DENS = DISPERSION JET FLUID DENSITY, KG/M**3
C      TO = AMBIENT TEMPERATURE, DEGREES RANKINE
C      ACCLASS(J) = FLOW REGIME DESCRIPTION
C      DIAJET = INITIAL PLUME DIAMETER, CM
C      TESTNO = EXPERIMENTAL TEST NUMBER
C      QINIT = INITIAL PLUME FLOWRATE, M**3/S
C      SPTIME = TOTAL TIME OF SPILL, S
C      TIMINC = TIME INCREMENT, S
C      TIMMAX = MAXIMUM TIME OF THE SPILL EVALUATION, S
C      WC = WIDTH OF THE CHANNEL, M
C      DC = DEPTH OF THE CHANNEL, M
C      XOBS = DOWNSTREAM DISTANCE TO THE OBSERVATION POINT, M
C      YOBS = Y DIMENSION FROM THE CENTER OF THE CHANNEL TO THE
C             OBSERVATION LOCATION, M
C      ZOBS = Z DIMENSION FROM THE CHANNEL SURFACE TO THE OBSERVATION
C             LOCATION, M (FOR THE PLUME CENTERLINE CONCENTRATION, SET
C             ZOBS=-1.0)
C      ALOC = DISTANCE IN THE Y DIRECTION FROM THE CHANNEL CENTERLINE TO
C             THE SPILL ORIGIN, M
C      BLOC = VERTICAL DISTANCE FROM THE CHANNEL SURFACE TO THE SPILL
C             ORIGIN, M
C      KNF = NEAR FIELD MODEL DECAY RATE COEFFICIENT
C      KIF = INTERMEDIATE FIELD MODEL DECAY RATE COEFFICIENT
C      KFF = FAR FIELD MODEL DECAY RATE COEFFICIENT
C      EYCOEF = Y TURBULENCE COEFFICIENT FOR THE NEAR FIELD MODEL
C      EZCOEF = Z TURBULENCE COEFFICIENT FOR THE NEAR FIELD MODEL
C      SLCONC = ERROR IN MATCHING THE NEAR FIELD AND INTERMEDIATE FIELD
C             CONCENTRATIONS AT THE POINT OF CONVERSION
C      XLSINC = DISTANCE INCREMENT FOR THE INTERMEDIATE FIELD MODEL
C             MATCHING ROUTINE, M
C      UR = MEAN RIVER VELOCITY, M/S
C      K1 = INITIAL JET DIRECTION INDICATOR(+1=HORIZONTAL DOWNSTREAM,
C             -1=HORIZONTAL UPSTREAM, 0=ALL OTHER CONDITIONS)
C      K2 = INITIAL JET DIRECTION INDICATOR(+1=VERTICAL UPWARD, -1=
C             VERTICAL DOWNWARD, 0=ALL OTHER CASES)
C      K3 = INITIAL JET DIRECTION INDICATOR(+1=HORIZONTAL TRANSVERSE
C             TO THE RIGHT, -1=HORIZONTAL TRANSVERSE TO THE LEFT, 0=
C             ALL OTHER CASES)
C
C DIMENSIONS:
C

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INTEGER COUNT, RUNGE, HAMING
REAL KNF, KIF, KFF, LAM, MASS, LOC, JAY
DOUBLE PRECISION ACLAS8(4), TESTNO(1)
DIMENSION TE(6), YR(6), FR(6), Y(4,6), F(3,6), YRS(6), LOC(5,2)
DIMENSION ERFN(4), ERFI(4), ERFF(4)
DIMENSION XOD(10), ZOD(10), PATHL(10)
COMMON/PHYS/DCDR, EPS, UPRI, ROA, DENS, G, UR, UA
COMMON/HQS1/C1, C2, C3, C4, C5, C6, DPLU
COMMON/HQS2/AFM1, AFM12, DELRO, CA, Z0, B2M1, CAI
COMMON/CON2/ROT, ALFA1, ALFA2, ALFA3

C
C***** READ IN DATA FROM FILE 'SPILLIN.DAT' ****
OPEN(UNIT=1, NAME='SY0: SPILLIN.DAT', 0, READONLY, TYPE='OLD')

READ(1,600) X, H, DISTA, DISTAN
READ(1,601) ROA, DENS, TO, UR
READ(1,602) TESTNO(1)
READ(1,603) (ACCLASS(J), J=1, 4)
READ(1,604) DIAJET, QINIT, SPTIME
READ(1,605) TIMINC, TIMMAX
READ(1,606) WC, DC, ALOC, BLOC
READ(1,607) KNF, KIF, KFF
READ(1,608) EYCOEF, EZCOEF, SLCONC, XLSINC
READ(1,609) K1, K2, K3

C
C***** PRINT HEADINGS AND VALUES OF PARAMETERS AND INITIAL CONDITIONS *
WRITE(3,717)
WRITE(3,708) TESTNO(1)
WRITE(3,709) (ACCLASS(J), J=1, 4)
WRITE(3,704) DISTA, DISTAN
WRITE(3,736) ROA, DENS, TO, DIAJET, TLV
WRITE(3,705) QINIT, TPER, SPTIME, TIMINC, TIMMAX, WC, DC
WRITE(3,706) ALOC, BLOC, KNF, KIF, KFF, LAM
WRITE(3,707) CONC, SLCONC, XLSINC
WRITE(3,712) UR
IF (K1, EQ, 1) WRITE(3,751)
IF (K1, EQ, -1) WRITE(3,752)
IF (K2, EQ, 1) WRITE(3,753)
IF (K2, EQ, -1) WRITE(3,754)
IF (K3, EQ, 1) WRITE(3,755)
IF (K3, EQ, -1) WRITE(3,756)
WRITE(3,735) EYCOEF, EZCOEF
WRITE(3,719) ALFA1, ALFA2, ALFA3
WRITE(3,726)
WRITE(3,711)

C
C***** INITIALIZE VARIABLES AND ASSIGN VALUES TO CONSTANTS
G= 9.80665
XINIT= X
TLV= 0.05
ALFA1= 0.0570
ALFA2= 0.500
ALFA3= 0.001
LAM= 1.16190
CONC= 0.3679
EPS= 0.000000001
PI= 3.141592654
NUMINC=-10.0
NUMIN=0
IAQ= 0
ALTL=ALFA3*TLV
IF (ALTL, EQ, 0.0) GO TO 998
UPRI=UR*TLV

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C..... IF A VALUE FOR H, THE INTEGRATION STEPSIZE, HAS NOT BEEN
C..... INPUT, THEN SET H=0.01*DIAJET/3.0. .....
IF (H.LE.0.001) H= DIAJET*0.002
HH= H
IF (ROA.EQ.DENS) DCDR=1.0E+20
IF (ROA.EQ.DENS) GO TO 4
DCDR=1. / (1. -ROA/DENS)
4 ROT=(1. -ROA/DENS)/ROA
MASS=QINIT*DENS
XEND=UR*SPTIME
STM=SPTIME

C
C**** CALCULATE HYDRAULIC CHARACTERISTICS OF THE RIVER ****
C..... CALCULATE RH-HYDRAULIC RADIUS OF THE CHANNEL. .....
RATWD= WC/DC
RH=(WC*DC)/(2.0*DC+WC)
IF (RATWD.GT.100.0) RH=DC
C..... CALCULATE THE VALUE OF UST, THE FRICTION VELOCITY. .....
C..... IF 0.5.LT.EYCOEF.LT.0.7, THEN ASSUME A RIVER FLOW. .....
IF (EYCOEF.GE.0.5.AND.EYCOEF.LE.0.7) GO TO 7
C..... ASSUME A CHANNEL FLOW TO CALCULATE UST. .....
UST= 0.03426*UR/(RH**0.16667)
GO TO 10
C..... ASSUME A RIVER FLOW TO CALCULATE UST. .....
7 UST= 0.0952*UR/(RH**0.16667)
10 CONTINUE
C..... CALCULATE VALUES FOR THE VERTICAL, CROSS-STREAM AND THE
C..... LONGITUDINAL DIFFUSION COEFFICIENTS IN THE NEAR FIELD.
C..... INTERMEDIATE FIELD, AND THE FAR FIELD. .....
EZNF= EZCOEF*DC*UST
EYNF= EYCOEF*DC*UST
EXNF= EYNF
EYIF= EYNF
EXIF= 5.93*DC*UST
EXFF= 0.18*((UR*UST)**0.5)*(WC*WC)/RH
C..... CALCULATE THE VALUE OF ZR FOR THE LOG VELOCITY PROFILE. .....
C..... REQUIRE A FIT TO UR AT Z=ZO=DC. .....
VK= 0.4
U0= UR
ZO= DC
ZR= ZO/(EXP(U0*VK/UST)-1.0)
C..... CALCULATE THE VALUE OF THE EXPONENT IN THE POWER LAW PROFILE. ..
C..... MATCH VALUES OF VELOCITY AT Z= 0.1*ZO. .....
UMATCH= (UST/VK)*LOG(1.0 + 0.1*ZO/ZR)
AF= (LOG(UMATCH/U0))/LOG(0.1)
C
C**** CALCULATE RIVER SPEED AT THE CHEMICAL PLUME DISCHARGE HEIGHT****
ZA=(DC-BLOC)/ZO
UA=U0*(ZA**AF)
C
C**** CALL SUBROUTINE JET TO CALCULATE THE INITIAL CONDITIONS FOR QOMS'
C**** PLUME MODEL INTEGRATION ****
C..... INITIALIZE VARIABLES FOR [VNF] MODEL. .....
13 DO 17 I=1,6
17 VR(I)=0.0
X= XINIT
YN(1)=DENS
CALL JET(YR,UA,QINIT,DIAJET,ROA,KK1,KK2,KK3,ALOC,BLOC,DC)
C..... VALUES OF YR2 THROUGH YR6 ARE DEFINED AND STORED FOR PRINTOUT
C..... IN SECTION 300. .....
YR2=YR(2)
YR3=YR(3)
YR4=YR(4)

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YR5=YR(5)
YR6=YR(6)
DO 20 I=1,6
TE(I)=0.0
Y(4, I)=YR(I)
F(1, I)=0.0
F(2, I)=0.0
F(3, I)=0.0
20 YRS(I)=0.0
COUNT = 0
IF (KK2. NE. 0) H=2.5*HH*(1.0-(DENS-ROA)/
1.0*KK2)*(ABS(YR(3))*(UR**2.0)**0.5)/(UR**1.50)
IF (KK2. EQ. 0) H=HH
AH=H
IF (IAQ.EQ.0) TYPE *, 'H', H
C
C**** CALCULATE THE DEVELOPMENT OF A BENT OVER PLUME WITH THE VERY NEAR
C**** FIELD (OMS') MODEL FOR PLUME CONCENTRATION, PLUME RADIUS, VELOC-
C**** ITY DECREMENT, AND PLUME ANGLE ****
IF (IAQ.EQ.0) TYPE *, ' BEGIN BENT OVER PLUME [VNF] MODEL '
C..... CALL RUNGE TO INTEGRATE FOR COUNT.LE.3. .....
100 IF (RUNGF(6,YR,FR,X,H).NE.1) GO TO 114
C..... CALL RHS TO CALCULATE RIGHT HAND SIDES. .....
CALL RHS(YR,YRS)
DO 101 K=1,4
101 FR(K)=YRS(K)
FR(5)= COS(YR(4))
FR(6)= SIN(YR(4))
OO TO 100
114 COUNT = COUNT + 1
ISUB = 4 - COUNT
DO 117 J=1,6
117 Y(ISUB,J) = YR(J)
C..... CALCULATE RIVER SPEED AT THE DEPTH OF THE CHEMICAL PLUME. .....
ZA= (DC+YR(6))/Z0
UA= U0*(ZA**AF)
CALL RHS(YR,YRS)
DO 120 K=1,4
120 F(ISUB,K)=YRS(K)
F(ISUB,5)= COH(YR(4))
F(ISUB,6)= SIN(YR(4))
123 CONTINUE
IF (COUNT.LE.3) OO TO 133
IF (ARS(Y(1,1)).LT. DENS/3.0) H=AMAX1(HH, H)
IF ((DENS-ROA)*K2.GT.0.0. AND. Y(1,1).GT. DENS) OO TO 127
IF ((DENS-ROA)*K2.GT.0.0. AND. Y(1,1).LT. 0.0) OO TO 127
OO TO 129
127 K1=1
K2=0
WRITE(3,715)
TYPE *, 'JET DIRECTION CHANGED.
OO TO 13
129 CONTINUE
C..... TEST WHETHER X0BS IS IN THE VERY NEAR FIELD REGION. .....
C..... IF SO, TRANSFER TO BLOCK 320 FOR OUTPUT. .....
C..... IF NOT, CONTINUE THE VNF MODEL COMPUTATIONS. .....
IF (IAQ.EQ.1. AND. Y(1,5).GT. X0BS) OO TO 320
IF (IAQ.EQ.1. AND. Y(1,5).LT. X0BS) OO TO 130
C
C**** IF X.LE. DISTA, PRINT X AND Y LOCATION AND PLUME CENTERLINE CON-
C**** CENTRATION VALUES... RESET DISTA=DISTA+DISTAN ****
C..... [CALCULATION OF CENTERLINE CONCENTRATION INCLUDES THE EFFECT OF
C..... IMAGES ABOUT THE TOP AND BOTTOM SURFACES OF THE RIVER]. .....

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AROT= (2.*(-Y(1,6))/(LAM*Y(1,2)))**2
ARGB= (2.*(DC+Y(1,6))/(LAM*Y(1,2)))**2
YCL=Y(1,1)*(1.+EXP(-AROT)+EXP(-ARGB))
IF (IAG.EQ.0. AND. Y(1,5).GE. DISTA) WRITE(3,734) Y(1,5),-Y(1,6),
1YCL
IF (IAG.EQ.0. AND. Y(1,5).GE. DISTA) DISTA=DISTA+DISTAN
130 CONTINUE
C
C***** IF PLUME CENTERLINE IS ABOVE THE CHANNEL FLOOR, GO TO 131 *****
IF (DC+Y(1,6).GT.0.01*DC) GO TO 131
C..... IF PLUME IS ON THE CHANNEL FLOOR, TEST FOR FROUDE NUMBER.....
FROUDE= ROA*UA*UA/(DENS-ROA)*Q*DIAJET*0.01
C..... IF FROUDE. LT. 0., PLUME WILL RISE, GO TO 132.....
IF (FROUDE. LT. 0.) GO TO 132
C..... IF FROUDE. GT. 25., PLUME WILL BE NEUTRALLY BUOYANT, GO TO 132.
IF (FROUDE. GT. 25.) GO TO 132
C..... FOR 25.GT.FROUDE.GT.0., GRAVITY SPREADING IS POSSIBLE.....
C..... SET ZPLUCL=DC, AND GO TO 200.....
ZPLUCL=DC
GO TO 200
131 CONTINUE
C
C***** IF PLUME CENTERLINE IS BELOW THE CHANNEL SURFACE, GO TO 132*****
IF (DC+Y(1,6).LT.0.99*DC) GO TO 132
C..... IF PLUME IS ON THE SURFACE, TEST FOR FROUDE NUMBER.....
FROUDE= ROA*UA*UA/(DENS-ROA)*Q*DIAJET*0.01
C..... IF FROUDE. GT. 0., PLUME WILL FALL, GO TO 132.....
IF (FROUDE. GT. 0.) GO TO 132
C..... IF FROUDE. LT. -25., PLUME WILL BE NEUTRALLY BUOYANT, GO TO 132..
IF (FROUDE. LT. -25.) GO TO 132
C..... FOR 0.GT.FROUDE.GT.-25., GRAVITY SPREADING IS POSSIBLE.....
C..... SET ZPLUCL=0.0, AND GO TO 200.....
ZPLUCL=0.0
GO TO 200
132 CONTINUE
C
C***** IF THE PLUME FILLS THE CHANNEL, GO TO 300 AND USE THE NEAR
C***** FIELD POINT SOURCE MODEL EQUATIONS. ****
RC= LAM*Y(1,2)*(-ALOG(CONC))*0.5
IF (2.0*RC.GT.DC) GO TO 300
IF (2.0*RC.GT.WC) GO TO 300
C
C***** IF THE PLUME CONCENTRATION IS VERY DILUTE, GO TO 300 AND USE THE
C***** NEAR FIELD POINT SOURCE MODEL EQUATIONS*****
IF (Y(1,1).LT.0.00001*DENS) GO TO 300
133 CONTINUE
IF (COUN1.LT.3) GO TO 100
C..... FOR COUNT.GT.3 CALL HAMING TO CONTINUE INTEGRATION OF THE
C..... PLUME MODEL EQUATIONS.....
137 M = HAMING(6,Y,F,X,H,TE)
DO 140 K=1,4
140 YR(K)=Y(1,K)
C..... CALCULATE RIVER SPEED AT THE DEPTH OF THE CHEMICAL PLUME.....
ZA= (DC+Y(1,6))/Z0
UA= U0*(ZA**AF)
C..... CALL RHS TO CALCULATE THE RIGHT HAND SIDES.....
CALL RHS(YR,YRS)
DO 143 K=1,4
143 F(1,K)=YRS(K)
F(1,5)=COS(Y(1,4))
F(1,6)=SIN(Y(1,4))
IF (M.EQ.1) GO TO 137
C..... INCREMENT STEP COUNTER AND CONTINUE INTEGRATION.....

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COUNT= COUNI+1
IF (Y(1,6).GT.0.0) Y(1,6)=0.0
IF (Y(1,6).LT.-DC) Y(1,6)=-DC
00 TO 123
200 CONTINUE
C
C***** CALCULATE THE DEVELOPMENT OF THE CHEMICAL PLUME ABOVE OR BELOW
C***** A FREE SURFACE WITH THE VERY NEAR FIELD (COLENBRANDER'S) MODEL
C***** FOR PLUME CONCENTRATION, PLUME WIDTH AND VERTICAL AND CROSS-
C***** STREAM DISPERSION COEFFICIENTS ****
XCONV=Y(1,5)
ZCONV=Y(1,6)
CVCON=Y(1,1)
XSTART=0.0
XPS=0.0
C..... WRITE OUT THE LAST VALUES COMPUTED BY OOMS MODEL (TO COMPLETE
C..... LISTING FOR X=DISTAN).....
IF (IAQ.EQ.0) WRITE(3,734) Y(1,5),-Y(1,6),Y(1,1)
IF (IAQ.EQ.0) WRITE(3,780)
IF (IAQ.EQ.0) WRITE(3,781)
IF (IAQ.EQ.0) TYPE *, ' BEGIN GRAVITY SPREADING [VNF] MODEL '
C..... CALCULATE VALUES FOR THE CONSTANTS NEEDED FOR COLENBRANDER'S
C..... MODEL.....
H=H*5.0
AF1 =AF+1.0
AFM1 =1./AF1
AFM12=0.5-AF
QAM =1.087743
QAMRT= SQRT(QAM)
PI2R =SQRT(PI/2)
BTA = 0.500
DLA= SQRT(2.0*EYNF/U0)
BM1 = 1./BTA
B2M1= 2.0-B11
DELRO= (DENS-ROA)/DENS
CA= 2.*Y(1,1)
DPLU= ROA + CA*DELRO
CA6 =8.*BTA/PI
CVO = DLA*SQRT(2.)
CBEFF=0.3*SQR(PI)
C1 = VK*UST*AF1*AF1/(Z0*U0)
C2 = QAM/AF1
IF (DENS.GT.ROA) C3=Q*(DPLU-ROA)/(ROA*UST*UST)
IF (DENS.LT.ROA) C3=Q*(ROA-DPLU)/(ROA*UST*UST)
C4 = DPLU*U0*Z0/AF1
IF (DENS.GT.ROA) C5= QAM*QAMRT*SQRT(Q*Z0/(U0*U0*AF1))
IF (DENS.LT.ROA) C5= QAMRT*SQRT(Q*Z0/(U0*U0*AF1))
C6 = CA6*(DLA*PI2R)**BM1
C..... CALCULATE THE VALUE OF THE DENSIMETRIC FROUDE NUMBER.....
FROUDE= ROA*U0*U0/(ABS(DENS-ROA)*G*DIAJET*0.01)
C..... IF ABS(FROUDE).LT.0.6, SWITCH TO THE POOL SPREADING MODEL.....
IF (ABS(FROUDE).LT.0.6) 00 TO 204
C..... USE THE POOL SPREADING MODEL.....
C..... COMPUTE THE EQUILIBRIUM SIZE OF THE DENSE CHEMICAL POOL.....
C..... CALCULATE MASS FLOWRATE OF DILUTE CHEMICAL SOLUTION INTO THE
C..... POOL FROM A MASS BALANCE BASED UPON THE VALUE OF CA.....
QMIN= DENS*QINIT*(DELRO+ROA/CA)
C..... CALCULATE THE RATE OF MASS UPTAKE FROM THE POOL.....
XS= 0.0
C..... INITIALIZE VARIABLES.....
C..... DEFINE.....
C..... SA= (S2/Z0)**AF1.....
C..... SR= C1/APHI.....

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SA= 0.0
APHI= 0.62
SR= C1/APHI
C.....CALL RUNGE TO INTEGRATE EQUATION FOR (SZ/Z0)**AF1.....
201 IF (RUNGE(1,SA,SR,XS,H).NE. 1) GO TO 202
SZ= Z0*(SA**AFM1)
HEFF= C2*SZ
RICH= C3*HEFF
APHI= 0.62 + 1.3911*(RICH**0.7)
C.....UPDATE RIGHT HAND SIDE FOR RUNGE.....
SR= C1/APHI
GO TO 201
202 CONTINUE
SZ= Z0*(SA**AFM1)
HEFF= C2*SZ
RICH= C3*HEFF
APHI= 0.62 + 1.3911*(RICH**0.7)
SR= C1/APHI
C.....CALCULATE MASS UPTAKE RATE USING COLENBRANDER'S EQUATION.....
QMINOT= C4*SA/XS
QMDOT= QMDOT*XS*XS
IF (QMIN.GT.QMDOT) GO TO 201
C.....SET INITIAL VALUES OF COLENBRANDER VARIABLES.....
YR(1)= SA
B= 0.5*XS
SY= 0.0
YR(2)= B
YR(3)= SY
X= Y(1,5) + 0.5*XS
GO TO 205
C.....MATCH THE OOMS' MODEL PLUME PROFILE TO COLENBRANDER'S PLUME
C.....PROFILE.....
204 CONTINUE
YR(3)=0.
YR(2)= CBEFF*LAM*Y(1,2)
SZ= YR(2)/CAM
YR(1)= (SZ/Z0)**AF1
205 CONTINUE
C.....INITIALIZE STEP COUNTER AND FIRST ROW OF Y MATRIX IN PREPARA-
C.....TION FOR INTEGRATION OF COLENBRANDER'S PLUME MODEL EQUATIONS.....
CCA= (CA)*YR(1)*YR(2)
INT = 10
COUNT = 0
DO 206 J=1,3
TE(J) = 0.
206 Y(4,J) = YR(J)
C.....CALL RUNGE TO INTEGRATE ACROSS THE FIRST THREE STEPS.....
208 IF (RUNGE(3,YR,FR,X,H).NE. 1) GO TO 210
C.....RICHARDSON NUMBER DEPENDS UPON LOCAL VALUE OF CONCENTRA-
C.....TION, HENCE UPDATE CA, DPLU AND C3 WHEN CALLING RHS2.....
CA= CCA/(YR(1)*YR(2))
DPLU= ROA + DFLRO*CA
IF (DENS.GT.ROA) C3=0.0*(DPLU-ROA)/(ROA*UST*UST)
IF (DENS.LT.ROA) C3=0.0*(ROA-DPLU)/(ROA*UST*UST)
C.....CALL RHS2 TO CALCULATE THE RIGHT HAND SIDES FOR THE NEXT STEP...
CALL RHS2(YR,YRS)
DO 209 K=1,3
209 FR(K)= YRS(K)
GO TO 208
210 COUNT = COUNT + 1
C.....COMPUTE VALUES OF THE PRIMARY VARIABLES.....
CA = CCA/(YR(1)*YR(2))
SY = SQRT(YR(3))

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B = YR(2) - CBEFF*SY
SZ = (YR(1)++AFM1)*Z0
ISUB = 4 - COUNT
C..... TRANSFER COMPUTED VALUES FROM RUNGE INTO Y AND F MATRICES..
C..... TO PROVIDE INITIAL DATA NEEDED BY HAMING. .....
DO 213 J=1,3
213 Y(ISUB,J) = YR(J)
C..... RICHARDSON NUMBER DEPENDS UPON LOCAL VALUE OF CONCENTRA-
C..... TION, HENCE EVALUATE CA, DPLU AND C3 INCLUDING EFFECT OF
C..... SIDEWALL IMAGES ON CENTERLINE CONCENTRATION. .....
ARQ1= (WC-2*ALOC-B)/SY
ARQ12=(2*WC-B)/SY
IF (ARQ1.LT.0.0) ARQ1=0.
IF (ARQ12.LT.0.0) ARQ12=0.
ASQ1=ARQ1*ARQ1
ASQ12=ARQ12*ARQ12
ARQ2= (WC+2*ALOC-B)/SY
ARQ22=(2*WC-B)/SY
IF (ARQ2.LT.0.0) ARQ2=0.
IF (ARQ22.LT.0.0) ARQ22=0.
ASQ2=ARQ2*ARQ2
ASQ22=ARQ22*ARQ22
CIMAGE= CA*(EXP(-ASQ1) + EXP(-ASQ12) + EXP(-ASQ2) + EXP(-ASQ22))
CAI= CA + CIMAGE
DPLU=ROA+CA*DELRO
IF (DENS.GT.ROA) C3=Q*(DPLU-ROA)/(ROA*UST*UST)
IF (DENS.LT.ROA) C3=Q*(ROA-DPLU)/(ROA*UST*UST)
C..... CALL RHS2 TO CALCULATE THE RIGHT HAND SIDES FOR THE NEXT STEP...
CAJL RHS2(YH,YRS)
DO 217 K=1,3
217 F(ISUB,K)=YRS(K)
C..... PRINT VALUES OF PLUME CENTERLINE CONCENTRATION, DISPERSION
C..... COEFFICIENTS, AND PLUME WIDTH WHENEVER X= DISTA. .....
220 CONTINUE
IF (COUNT.LE.3) GO TO 223
CA = CCA/(Y(1,1)*Y(1,2))
SY = SQRT(Y(1,3))
B = Y(1,2) - CBEFF*SY
SZ= (Y(1,1)++AFM1)*Z0
C..... INCLUDE EFFECT OF SIDEWALL IMAGES ON CENTERLINE CONCENTRATION
ARQ1= (WC-2*ALOC-B)/SY
ARQ12=(2*WC-B)/SY
IF (ARQ1.LT.0.0) ARQ1=0.
IF (ARQ12.LT.0.0) ARQ12=0.
ASQ1=ARQ1*ARQ1
ASQ12= ARQ12*ARQ12
ARQ2= (WC+2*ALOC-B)/SY
ARQ22=(2*WC-B)/SY
IF (ARQ2.LT.0.0) ARQ2=0.
IF (ARQ22.LT.0.0) ARQ22=0.
ASQ2= ARQ2*ARQ2
ASQ22=ARQ22*ARQ22
CIMAGE= CA*(EXP(-ASQ1) + EXP(-ASQ12) + EXP(-ASQ2) + EXP(-ASQ22))
CAI= CA + CIMAGE
C..... TEST WHETHER X0BS IS IN THE VERY NEAR FIELD REGION. .....
C..... IF SO, TRANSFER TO BLOCK 350 FOR OUTPUT. .....
C..... IF NOT, CONTINUE THE VNF MODEL COMPUTATION. .....
IF (IAQ.EQ.1.AND.X.GT.X0BS) GO TO 350
IF (IAQ.EQ.1.AND.X.LT.X0BS) GO TO 223
IF (X.LT.DISTA) GO TO 223
WRITE(3,709) X,CAI,SY,SZ,B,Y(1,2)
DISTA=DISTA + DISTAN
223 CONTINUE

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C.....SWITCH TO THE INTERMEDIATE FIELD MODEL WHEN (SZ GE. 0. 5*DC)...
  IF (SZ.GE.0.5*DC) GO TO 270
  IF ( COUNT.LT.3 ) GO TO 208
C.....CALL HAMING TO INTEGRATE THE PLUME MODEL EQUATIONS. .....
  227 M = HAMING(3,Y,F,X,H,TE)
  DO 230 K=1,3
  230 YR(K)=Y(1,K)
C.....RICHARDSON NUMBER DEPENDS UPON LOCAL VALUE OF CONCENTRA-
C.....TION, SO EVALUATE CA, DPLU AND C3 INCLUDING EFFECT OF
C.....SIDEWALL IMAGES. .....
  DPLU= ROA + CA*DELRO
  IF (DENS.GT.ROA) C3=G*(DPLU-ROA)/(ROA*UST*UST)
  IF (DENS.LT.ROA) C3=G*(ROA-DPLU)/(ROA*UST*UST)
C.....CALL RHS2 TO CALCULATE THE RIGHT HAND SIDES FOR THE NEXT STEP
  CALL RHS2(YR,YRS)
  DO 233 K=1,3
  233 F(1,K)=YRS(K)
  IF (M.EQ.1) GO TO 227
C.....INCREMENT STEP COUNTER AND CONTINUE INTEGRATION. .....
  COUNT = COUNT + 1
C.....CALCULATE B AND TEST WHETHER B.LE.0.?
C.....IF SO, GO TO 237. .....
  B = Y(1,2) - CBEFF*SY
  IF (B.LT.0.) GO TO 237
  GO TO 270
  237 CONTINUE
C.....FOR B=0, USE A SIMPLIFIED SET OF PLUME MODEL EQUATIONS. .....
C.....CALCULATE THE VIRTUAL ORIGIN DISTANCE FOR SY, RESET
C.....THE INTEGRATION COUNTER, AND NEGLECT FURTHER GRAVITY
C.....SPREADING OF THE CHEMICAL PLUME. .....
  B= 0.
  XV = (SY/CVO)**BM1 - X
C.....CALCULATE SY AS IF FOR A POINT SOURCE. .....
C.....INCREASE STEP SIZE TO REDUCE COMPUTING TIME. .....
  H= 10.*H
  COUNT = 0
  TE2 = 0.
  YF = Y(1,1)
C.....CALL RUNGE TO INTEGRATE ACROSS THE FIRST THREE STEPS. .....
  240 IF (RUNGE(1,YF,FF,X,H).NE.1) GO TO 243
  SY = CVO*(X+XV)**BTA
  SZ = ZO*(YF**AFM1)
  BEFF = CBEFF*SY
  CA = CCA/(YF*BEFF)
C.....RICHARDSON NUMBER DEPENDS UPON THE LOCAL VALUE OF CONCENTRA-
C.....TION, HENCE EVALUATE CA, DPLU AND C3. .....
  DPLU= ROA + CA*DELRO
  IF (DENS.GT.ROA) C3=G*(DPLU-ROA)/(ROA*UST*UST)
  IF (DENS.LT.ROA) C3=G*(ROA-DPLU)/(ROA*UST*UST)
  HEFF=C3*SZ
  RICH=C3*HEFF
  APHI= 0.62 + 1.3911*(RICH**0.7)
C.....COMPUTE THE RIGHT HAND SIDE FOR RUNGE. .....
  FF= C1/APHI - YF*BTA/(X+XV)
  GO TO 240
C.....TRANSFER COMPUTED VALUES FROM RUNGE INTO Y AND F MATRICES TO
C.....PROVIDE THE INITIAL DATA NEEDED BY HAMING. .....
  243 COUNT = COUNT + 1
  ISUB = 4 - COUNT
  Y(ISUB,1) = YF
C.....COMPUTE VALUES OF THE PRIMARY VARIABLES. .....
  SY = CVO*((X+XV)**BTA)
  SZ = ZO*(YF**AFM1)

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```

BEFF= CBEFF+SY
CA = CCA/(YF*BEFF)
C..... RICHARDSON NUMBER DEPENDS UPON THE LOCAL VALUE OF CONCENTRA-
C..... TION, HENCE EVALUATE CA, DPLU AND C3.
DPLU = ROA + CA*DELRO
IF (DENS. GT. ROA) C3=C*(DPLU-ROA)/(ROA*UST*UST)
IF (DENS LT. ROA) C3=C*(ROA-DPLU)/(ROA*UST*UST)
HEFF=C2*SZ
RICH= C3*HEFF
APHI= 0.62 + 1.3911*(RICH**0.7)
C..... COMPUTE THE RIGHT HAND SIDE FOR INPUT TO HAMING.
FF= C1/APHI - YF*BTA/(X+XV)
F(ISUB,1) = FF
247 CONTINUE
C..... PRINT VALUES OF PLUME CENTERLINE CONCENTRATION, DISPERSION
C..... COEFFICIENTS, AND PLUME WIDTH WHENEVER X= DISTA.
IF (IAQ EQ. 0. AND. X. LT. DISTA) GO TO 250
IF (COUNT. LE. 3) GO TO 250
C..... COMPUTE VALUES OF THE PRIMARY VARIABLES.
SY = CVO*((X+XV)**BTA)
BEFF= CBEFF+SY
CA = CCA/(Y(1,1)*BEFF)
SZ = Z0*(Y(1,1)**AFM1)
C..... INCLUDE EFFECT OF SIDEWALL IMAGES ON CENTERLINE CONCENTRATION
ARG1=((WC-2*ALOC)/SY)**2
ARG12=((2*WC)/SY)**2
ARG2=((WC+2*ALOC)/SY)**2
ARG22=((2*WC)/SY)**2
CIMAGE= CA*(EXP(-ARG1)+EXP(-ARG12)+EXP(-ARG2)+EXP(-ARG22))
CAI= CA + CIMAGE
C..... TEST WHETHER X0BS IS IN THE VERY NEAR FIELD REGION.
C..... IF SO, TRANSFER TO BLOCK 350 FOR OUTPUT.
C..... IF NOT, CONTINUE THE VNF MODEL COMPUTATION.
IF (IAQ EQ. 1. AND. X. GT. X0BS) GO TO 350
IF (IAQ EQ. 1. AND. X. LT. X0BS) GO TO 250
WRITE(3,788) X,CAI,SY,SZ,B,BEFF
DISTA= DISTA + DISTAN
250 CONTINUE
C..... RICHARDSON NUMBER DEPENDS UPON LOCAL VALUE OF CONCENTRA-
C..... TION, HENCE EVALUATE CA, DPLU AND C3.
CA= CCA/(Y(1,1)*BEFF)
DPLU= ROA + CA*DELRO
IF (DENS. GT. ROA) C3=C*(DPLU-ROA)/(ROA*UST*UST)
IF (DENS. LT. ROA) C3=C*(ROA-DPLU)/(ROA*UST*UST)
SZ= Z0*(Y(1,1)**AFM1)
HFF= C2*SZ
RICH= C3*HEFF
APHI= 0.62 + 1.3911*(RICH**0.7)
C..... SWITCH TO THE INTERMEDIATE FIELD MODEL IF (SZ. GE. 0.5*DC).
IF (SZ.GE. 0.5*DC) GO TO 270
IF (COUNT. LT. 3) GO TO 240
C..... CALL HAMING TO INTEGRATE ACROSS THE NEXT STEP.
253 M= HAMING(1,Y,F,X,H,TE)
SZ= Z0*(Y(1,1)**AFM1)
HFFF= C2*SZ
RICH= C3*HEFF
APHI= 0.62 + 1.3911*(RICH**0.7)
F(1,1) = C1/APHI - Y(1,1)*BTA/(X+XV)
IF (M. EQ. 1) GO TO 253
C..... INCREMENT STEP COUNTER AND CONTINUE INTEGRATION.
COUNT = COUNT + 1
GO TO 247
260 CONTINUE

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      WRITE(3, 787)
  270 CONTINUE
C***** TRANSITION TO THE INTERMEDIATE FIELD MODEL FROM COLENBRANDER'S
C***** VERY NEAR FIELD MODEL ****
C..... DEFINE XCLLS= DISTANCE FOR CONVERSION TO THE [IF] MODEL. .....
C..... XCLLS= X
C..... CALCULATE THE DISTANCE FOR CONVERSION TO THE [FF] MODEL. .....
C..... XXIF= 0.3*UR*WC*WC/EYNF
C..... WRITE OUT THE INITIAL CONDITIONS THAT WERE INPUT TO THE VNF...
C..... MODEL. .....
      WRITE(3, 702)
      WRITE(3, 710) UR, DENS, YR2, YR3, YR4, YR5, -YR6
C..... WRITE OUT THE FINAL CONDITIONS COMPUTED BEFORE TRANSFER TO. .....
C..... THE INTERMEDIATE FIELD MODEL. .....
      WRITE(3, 703)
      WRITE(3, 731) UR, CAI, B, BEFF, SY, SZ, X, ZPLUCL
C..... AVERAGE THE CONCENTRATION DISTRIBUTION FROM COLENBRANDER'S MODEL.
C..... OVER THE DEPTH OF THE CHANNEL TO GIVE AN EQUIVALENT STRENGTH FOR
C..... THE VERTICALLY AVERAGED LINE SOURCE INTERMEDIATE FIELD MODEL. .....
      TYPE *, ' BEGIN INTERMEDIATE FIELD [IF] LINE SOURCE MODEL.
      AVOC= 0.0
      DIV= DC/99.0
      CQSP= EXP(-KNF*XCLLS/UR)
C..... LEFT AND RIGHT IMAGES ARE INCLUDED IN CAI. .....
      DO 273 LI=1, 100
C..... PRIMARY PLUME. .....
      CQSP1= EXP(-((LI*DIV/SZ)**AF1))
C..... REFLECTION ABOUT THE OPPOSITE SURFACE. .....
      CQSP2= EXP(-(((2.*DC-LI*DIV)/SZ)**AF1))
      CQSP3= EXP(-(((2.*DC+LI*DIV)/SZ)**AF1))
C..... COMBINE TERMS. .....
      CQBM= CQSP*CAI*(CQSP1+CQSP2+CQSP3)
  273 AVOC= AVOC + CQBM
      AVOC= AVOC/100.
      GO TO 302
C
C***** NEAR FIELD POINT SOURCE MODEL ****
C..... DIFFUSION IN BOTH VERTICAL AND CROSS STREAM DIRECTIONS. .....
C..... CALCULATE THE LOCATION OF THE STREAMWISE ORIGIN FOR THE. .....
C..... NEAR FIELD MODEL. .....
      300 CONTINUE
      TYPE *, ' BEGIN NEAR FIELD [NF] POINT SOURCE MODEL.
      XCONV=Y(1, 5)
      ZCONV=Y(1, 6)
      CVCON=Y(1, 1)
C..... WRITE OUT THE LAST VALUES COMPUTED IN OOMS' MODEL. .....
C..... (TO COMPLETE THE LISTING OF VALUES WHEN X= DISTAN).....
      WRITE(3, 734) Y(1, 5), -Y(1, 6), Y(1, 1)
C..... WRITE OUT THE INITIAL CONDITIONS USED BY THE [VNF] MODEL. .....
      WRITE(3, 702)
      WRITE(3, 710) UR, DENS, YR2, YR3, YR4, YR5, -YR6
C..... WRITE OUT THE FINAL CONDITIONS AT TRANSFER FROM THE [VNF]. .....
C..... MODEL TO THE NEAR FIELD [NF] MODEL. .....
      WRITE(3, 703)
      WRITE(3, 710) UR, CVCON, Y(1, 2), Y(1, 3), Y(1, 4), Y(1, 5), -Y(1, 6)
      WRITE(3, 714) XX, AH, H
      WRITE(3, 727) EXNF, EYNF, EZNF, EXIF, EYIF, EXFF
      WRITE(3, 729) ALTL
C..... CALCULATE THE DISTANCE FROM A VIRTUAL ORIGIN FOR THE POINT. .....
C..... SOURCE MODEL THAT WILL GIVE A PLUME WITH THE SAME CROSS-.....
C..... SECTIONAL AREA AS OOMS' PLUME. .....
      XSTART=((LAM*LAM)*(Y(1, 2)*Y(1, 2))*UR)/(4.0*(EYNF*EZNF)**0.5)
      XPS=XSTART-XCONV

```

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C..... CALCULATE THE DISTANCE FOR CONVERSION TO THE [IF] MODEL. .....
  XCLLS=0. 3*UR*DC*DC/EZNF
C..... CALCULATE THE DISTANCE FOR CONVERSION TO THE [FF] MODEL. .....
C..... FROM THE POINT SOURCE MODEL ORIGIN. .....
  XXIF=0. 3*UR*WC*WC/EYNF
C..... AVERAGE THE CONCENTRATION DISTRIBUTION FROM THE [NF] MODEL. .....
C..... OVER THE DEPTH OF THE CHANNEL TO GIVE AN EQUIVALENT STRENGTH. .....
C..... FOR THE VERTICALLY AVERAGED LINE SOURCE [IF] MODEL. .....
  AVQC=0. 0
  DIV=DC/99. 0
  DO 301 LI=1, 100
    CPS1M=(MACS/(4. 0*PI*XCLLS*((EYNF-EZNF)**0. 5)))*
    1(EXP(-KNF*XCLLS/UR))
    CPSI1M=EXP(-(UR*((LI-1)*DIV)+Y(1, 6)**2. 0))/(4. 0*XCLLS*EZNF)
    CPSI2M=EXP((-(UR*((2. 0*ALOC-WC)**2. 0))/(4. 0*XCLLS*
    1EYNF))-(UR*((LI-1)*DIV)+Y(1, 6)**2. 0))/(4. 0*XCLLS
    2*EZNF))
    CPSI3M=EXP(-(UR*((LI-1)*DIV)-2. 0*DC-Y(1, 6)**2. 0))/(4. 0*XCLLS
    1*EZNF))
    CPSI4M=EXP((-(UR*((2. 0*ALOC+WC)**2. 0))/(4. 0*XCLLS*
    1EYNF))-(UR*((LI-1)*DIV)+Y(1, 6)**2. 0))/(4. 0*XCLLS
    2*EZNF))
    CPSI5M=EXP(-(UR*((LI-1)*DIV)-Y(1, 6)**2. 0))/(4. 0*XCLLS*EZNF)
    CPSM=CPS1M*(CPSI1M+CPSI2M+CPSI3M+CPSI4M+CPSI5M)
  301 AVQC=AVQC+CPSM
  AVQC=AVQC/100. 0
  TYPE *, ' BEGIN THE INTERMEDIATE FIELD [IF] LINE SOURCE MODEL.
  302 CONTINUE
C..... THIS SECTION DETERMINES THE DISTANCE FROM A VIRTUAL ORIGIN. .....
C..... FOR THE [IF] MODEL TO MATCH THE CONCENTRATION GIVEN BY THE. .....
C..... [NF] MODEL. .....
  MN=0
  XXLS=XLSINC
  304 TTLS=0. 0
  DO 307 IK=1, 20
    TLS1=COS(IK*PI*((WC/2. 0)+ALOC)/WC)
    TLS2=COS(IK*PI*((WC/2. 0)+ALOC)/WC)
    TLS3=EXP(-(IK**2)*(PI**2. 0)*EYIF*XXLS/(UR*(WC**2. 0)))
    TLS=TLS1*TLS2*TLS3
  307 TTLS=TTLS+TLS
  CCLLS=(MACS/(UR*DC*WC))*(1+2*TTLS)*(EXP(-KIF*XXLS/UR))
  RLSPS=CCLLS/AVQC
  IF (MN.EQ. 1) GO TO 310
  IF (MN.EQ. 2) GO TO 313
  IF (RLSPS.EQ. 1. 0) GO TO 317
  IF (RLSPS.LT. 1. 0) MN=1
  IF (RLSPS.LT. 1. 0) GO TO 310
  IF (RLSPS.GT. 1. 0) MN=2
  GO TO 313
  310 IF (RLSPS.LT. (1. 0-SLCONC)) XXLS=XXLS-XLSINC
  IF (RLSPS.LT. (1. 0-SLCONC)) GO TO 304
  GO TO 317
  313 IF (RLSPS.GT. (1. 0+SLCONC)) XXLS=XXLS+XLSINC
  IF (RLSPS.GT. (1. 0+SLCONC)) GO TO 304
  317 CONTINUE
  XFS=((UR*UR+4. 0*KFF*EXFF)**0. 5)*SPTIME)-(4. 0*((EXFF*SPTIME)
  1**0. 5))-(XCLLS-XXLS)
  XLS=XXLS-XCLLS+XPS
C..... THE CONDITIONS FOR TRANSITION TO AND FROM ALL MODELS ARE. .....
C..... COMPLETE. THE PROGRAM NOW PREPARES TO COMPUTE THE CONCEN-.....
C..... TRATION DISTRIBUTION AT USER SPECIFIED CO-ORDINATES. .....
C..... HERE, IAC IS SET = 1, IN PREPARATION FOR COMPUTATION. .....
C..... OF CONCENTRATION AT USER SPECIFIED LOCATIONS. .....

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IAC=1
IF (XSTART, EQ, 0.) GO TO 318
WRITE(3, 728) XCONV, XPS, CVCON
WRITE(3, 733) XCLLS-XPS, AVOC
WRITE(3, 737) XLS, RLSPS
WRITE(3, 747) XXIF-XLS, XFS-XXIF+XLS
TYPE *, ''
TYPE *, 'CONVERSION FROM VNF TO NF OCCURS AT X = ', XCONV, ' M'
TYPE *, ''
TYPE *, 'CONVERSION FROM NF TO IF OCCURS AT X = ', XCLLS-XPS, ' M'
TYPE *, ''
TYPE *, 'CONVERSION FROM IF TO FF OCCURS AT X = ', XXIF-XLS, ' M'
TYPE *, ''
CO TO 319
318 WRITE(3, 729) XCONV, ZPLUCL, CVCON
WRITE(3, 730) XCLLS, AVOC, XXLS, RLSPS
WRITE(3, 747) XXIF-XLS, XFS-XXIF+XLS
TYPE *, ''
TYPE *, 'CONVERSION FROM OOMS [VNF] MODEL TO COLENBRANDERS [VNF] '
TYPE *, 'MODEL OCCURS AT X= ', XCONV, ' M'
TYPE *, ''
TYPE *, 'CONVERSION FROM COLENBRANDERS [VNF] MODEL TO THE'
TYPE *, 'INTERMEDIATE [IF] MODEL OCCURS AT X= ', XCLLS, ' M'
TYPE *, ''
TYPE *, 'CONVERSION FROM [IF] TO [FF] OCCURS AT X= ', XXIF-XLS, ' M'
319 CONTINUF
XXCONV=XCONV
XXCLLS=XCLLS
XXPS=XPS
XLSS=XLS
XXIF=XXIF
XXFS=XFS
CO TO 417
320 CONTINU.
C..... X0BS LIES WITHIN THE [VNF] OF THE PLUME.
C..... THIS SECTION COMPUTES THE REQUIRED IMAGES WITH AN OBSERVER.
C..... LOCATED AT X0BS, Y0BS, AND Z0BS.
PLURAD=Y(1,2)*LAM*(-ALOC(CONC))**0.5
ID-1
IF (Z0BS, EQ, -1.0) ZZ0BS=-Y(1,6)
IF (Z0BS, EQ, -1.0) GO TO 323
ZZ0BS=Z0BS
323 COOM1=EXP(-((Y0BS-ALOC)*(Y0BS-ALOC)+(ZZ0BS+Y(1,6))*(ZZ0BS+
1Y(1,6)))/((LAM*LAM)*((Y(1,2))*(Y(1,2)))))

COOM2=EXP(-((Y0BS-WC+ALOC)*(Y0BS-WC+ALOC)+(ZZ0BS+Y(1,6))*(ZZ0BS+
1Y(1,6)))/((LAM*LAM)*((Y(1,2))*(Y(1,2)))))

COOM3=EXP(-((Y0BS-ALOC)*(Y0BS-ALOC)+(ZZ0BS-2.0*DC-Y(1,6))*(ZZ0BS-
1-2.0*DC-Y(1,6)))/((LAM*LAM)*((Y(1,2))*(Y(1,2)))))

COOM4=EXP(-((Y0BS+WC+ALOC)*(Y0BS+WC+ALOC)+(ZZ0BS+Y(1,6))*(ZZ0BS+
1Y(1,6)))/((LAM*LAM)*((Y(1,2))*(Y(1,2)))))

COOM5=EXP(-((Y0BS-ALOC)*(Y0BS-ALOC)+(ZZ0BS-Y(1,6))*(ZZ0BS-Y(1,6)))
1)/((LAM*LAM)*((Y(1,2))*(Y(1,2)))))

COOM=COOM1+COOM2+COOM3+COOM4+COOM5
CONCEN=Y(1,1)*COOM
GO TO 407
327 CONTINUE
C..... X0BS LIES WITHIN THE [NF] OF THE PLUME.
C..... THIS SECTION COMPUTES THE REQUIRED IMAGES WITH AN OBSERVER.
C..... LOCATED AT X0BS, Y0BS AND Z0BS.
CP81=(MASS/(4.0*PI*(X0BS+XPS)*((EYNF*EZNF)**0.5)))*
1(EXP(-KNF*(X0BS+XPS)/UR))
IF (Z0BS, EQ, -1.0) ZZ0BS=-ZCONV
IF (Z0BS, EQ, -1.0) GO TO 330

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ZZOBS=ZOBS
330 CPSM1=EXP((-(UR*((YOBS-ALOC)**2.0))/(4.0*(XOBS+XPS)*EYNF
1))-((UR*((ZZOBS+ZCONV)**2.0))/(4.0*(XOBS+XPS)*EZNF)))
CPSM2=EXP((-(UR*((YOBS+WC+ALOC)**2.0))/(4.0*(XOBS+XPS)*EYNF
1))-((UR*((ZZOBS+ZCONV)**2.0))/(4.0*(XOBS+XPS)*EZNF)))
CPSM3=EXP((-(UR*((YOBS-ALOC)**2.0))/(4.0*(XOBS+XPS)*EYNF
1))-((UR*((ZZOBS-2.0*DC-ZCONV)**2.0))/(4.0*(XOBS+XPS)*EZNF)))
CPSM4=EXP((-(UR*((YOBS+WC+ALOC)**2.0))/(4.0*(XOBS+XPS)*
1EYNF))-((UR*((ZZOBS+ZCONV)**2.0))/(4.0*(XOBS+XPS)*EZNF)))
CPSM5=EXP((-(UR*((YOBS-ALOC)**2.0))/(4.0*(XOBS+XPS)*EYNF
1))-((UR*((ZZOBS-ZCONV)**2.0))/(4.0*(XOBS+XPS)*EZNF)))
CONCEN=CPS1*(CPSM1+CPSM2+CPSM3+CPSM4+CPSM5)
GO TO 40
350 CONTINUE
C..... X0BS LIES WITHIN THE GRAVITY SPREADING REGION OF THE [VNF].
C..... THIS SECTION COMPUTES THE REQUIRED IMAGES WITH AN OBSERVER.
C..... LOCATED AT X0BS, Y0BS, AND Z0BS.
C..... VERTICAL PROFILE.
C..... IF ZPLUCL = DC, PLUME IS ON THE CHANNEL BOTTOM.
ZZOBS=ZOBS
IF (ZOBS, EQ, -1.0) ZZOBS=ZPLUCL
IF (ZPLUCL, LT, DC) GO TO 353
CVO= EXP(-((DC-ZZOBS)/SZ)**AF1)
CVI1=EXP(-((DC+ZZOBS)/SZ)**AF1)
GO TO 356
353 CONTINUE
C..... PLUME IS ON THE CHANNEL SURFACE.
CVO= EXP(-((ZZOBS)/SZ)**AF1)
CVI1=EXP(-((2*DC-ZZOBS)/SZ)**AF1)
356 CONTINUE
C..... CROSS-STREAM PROFILE.
C..... PRIMARY PLUME IS LOCATED AT Y=ALOC.
IF (ABS(ALOC-YOBS), GT, 8) GO TO 359
CCSO= 1.
GO TO 362
359 CCSO= EXP(-(((ABS(ALOC-YOBS)-8)/SY)**2))
362 CONTINUE
C..... FIRST IMAGE LOCATED AT Y= WC-ALOC.
IF (ABS(WC-ALOC-YOBS), GT, 8) GO TO 365
CCSI1= 1.
GO TO 368
365 CCSI1= EXP(-(((ABS(WC-ALOC-YOBS)-8)/SY)**2))
368 CONTINUE
C..... SECOND IMAGE LOCATED AT Y= -(WC+ALOC).
IF (ABS(-(WC+ALOC)-YOBS), GT, 8) GO TO 371
CCSI2= 1.
GO TO 374
371 CCSI2= EXP(-(((ABS(-(WC+ALOC)-YOBS)-8)/SY)**2))
374 CONTINUE
C..... THIRD IMAGE LOCATED AT Y= -(2WC-ALOC).
IF (ABS(-(2*WC-ALOC)-YOBS), GT, 8) GO TO 377
CCSI3= 1.
GO TO 380
377 CCSI3= EXP(-(((ABS(-(2*WC-ALOC)-YOBS)-8)/SY)**2))
380 CONTINUE
C..... FOURTH IMAGE LOCATED AT Y= (2*WC+ALOC).
IF (ABS((2*WC+ALOC)-YOBS), GT, 8) GO TO 383
CCSI4= 1.
GO TO 386
383 CCSI4= EXP(-(((ABS((2*WC+ALOC)-YOBS)-8)/SY)**2))
386 CONTINUE
C..... CALCULATE CONCENTRATION VALUE.
CONCEN= CA*(CVO+CVI1)*(CCSO+CCSI1+CCSI2+CCSI3+CCSI4)

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    GO TO 407
C..... XOBS LIES WITHIN THE [IFI].
C..... THIS SECTION COMPUTES THE CONCENTRATION WITH IMAGES.
C..... FOR A LINE SOURCE WITH DIFFUSION IN THE CROSS STREAM.
C..... DIRECTION.
    400 TTLS=0.0
      IF (ZOBS.EQ.-1.0) ZZOBS=-ZCONV
      IF (ZOBS.EQ.-1.0) GO TO 401
      ZZOBS=ZOBS
    401 DO 403 IM=1,20
C..... FIRST, THE COSINE TERM FOR THE SPILL LOCATION.
      TLS1=COS(IM*PI*((WC/2.0)+ALOC)/WC)
C..... NEXT, THE COSINE TERM FOR THE OBSERVER LOCATION.
      TLS2=COS(IM*PI*((WC/2.0)+YOBS)/WC)
C..... FINALLY, THE EXPONENTIAL DECAY TERM BELONGING TO THE.
C..... DOWNSTREAM DISTANCE FROM THE VIRTUAL ORIGIN.
      TLS3=EXP(-(IM**2)*(PI**2.0)*EYIF*(XOBS+XLS)/(UR*(WC**2.0)))
      TLS=TLS1*TLS2*TLS3
    403 TTLS=TTLS+TLS
      CONCEN=(MASS/(UR*DC*WC))*(1+2*TTLS)*(EXP(-KIF*(XOBS+XLS)/UR))
    407 IF(IC.NE.0) GO TO 410
      IF (ZOBS.EQ.-1.0) WRITE(3,738) XOBS,ZZOBS,TIMEE,WC/NUMINC
      IF (ZOBS.NE.-1.0) WRITE(3,739) XOBS,ZZOBS,TIMEE,WC/NUMINC
      IF (ID.EQ.1) WRITE(3,713) PLURAD
      IF (ID.NE.1) WRITE(3,718)
C..... SET IC EQUAL TO 1.
      IC=1
    410 WRITE(3,744) YOBS,CONCEN
    413 TIMEE=TIMEE+TIMINC
      IF (TIMEE.GT.TIMMAX) GO TO 417
      IF (TIMEE.GT.SPTIME) GO TO 800
      GO TO 407
    417 CONTINUE
C
C***** PREPARE TO ENTER ANOTHER SET OF OBSERVATION CO-ORDINATES*****
  IF (NUMIN.LE.NUMINC+1) TYPE *, 'XOBS= ',XOBS,' YOBS= ',YOBS,
  1' ZOBS= ',ZZOBS
  IF (NUMIN.LE.NUMINC) TYPE *, ''
  IF (NUMIN.LE.NUMINC) GO TO 420
  TYPE *, ''
  TYPE *, 'INPUT THE CONVERSION COORDINATES (XOBS, YOBS, ZOBS)'
  TYPE *, 'TO TERMINATE THE RUN, ENTER XOBS=-1.0 .'
  TYPE *, ''
  TYPE *, 'INPUT XOBS'
  ACCEPT *,XOBS
  TYPE *, ''
  IF (XOBS.EQ.-1.0) TYPE *, 'RUN TERMINATED'
  IF (XOBS.EQ.-1.0) GO TO 999
  TYPE *, 'INPUT ZOBS'
  TYPE *, 'INPUT ZOBS=-1.0 TO OBTAIN THE CENTERLINE OF THE PLUME'
  ACCEPT *, ZOBS
  TYPE *, ''
  TYPE *, 'ENTER THE NUMBER OF TRANSVERSE INCREMENTS'
  ACCEPT *, NUMINC
  TYPE *, ''
  NUMIN=0
  IC=0
  ID=0
  420 YOBS=(-WC/2.0)+NUMIN*(WC/NUMINC)
  NUMIN=NUMIN+1
  XCONV=XXCONV
  XCLLS=XXCLLS
  XPS=XXPS

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XLS=XLSS
XFS=XXFS
XXIF=XXIIF
TIMEE=0.0
423 IF (TIMEE*UR.LT.XOBS) TIMEE=TIMEE+TIMINC
IF (TIMEE*UR.LT.XOBS) GO TO 423
IF (TIMEE.GT.SPTIME) GO TO 800
C.....IS XOBS IN THE [VNF] REQUIRING DOMS' MODEL?.....
IF (XOBS.LE.XCONV) GO TO 13
C.....IS XOBS IN THE [VNF] REQUIRING COLENGRANDER'S MODEL?.....
IF (XSTART.EQ.0.0) GO TO 426
C.....IS XOBS IN THE [NF]?.....
IF (XOBS.LE.XCLLS-XPS) GO TO 327
C.....XOBS MUST BE IN THE [IF].....
GO TO 400
C.....IS XOBS IN THE [VNF] REQUIRING COLENGRANDER'S MODEL?.....
426 IF (XOBS.LE.XCLLS) GO TO 13
C.....XOBS MUST BE IN THE [IF]
GO TO 400
550 WRITE(3,744) STM, CONCEN
551 STM=STM+TIMINC
IF(STM.GT.TIMMAX) GO TO 417
XSPIL=STM*UR
C.....DETERMINE IF THE SPILL HAS REACHED THE OBSERVATION POINT.....
IF(XSPIL.LT.XOBS) GO TO 551
IF(XSPIL-XEND.GT.XOBS) GO TO 553
C.....DETERMINE THE CORRECT FLOW REGIME AT THE OBSERVATION POINT.....
XFLO=(XSPIL-XOBS)
C.....DETERMINE IF THE OBSERVATION POINT SEES THE [FF].....
IF (XXIFF.EQ.0.0) GO TO 595
IF (XEND-XFLO.GT.XIFF) GO TO 590
C.....DETERMINE IF THE OBSERVATION POINT SEES THE [IF].....
595 IF (XCLLS.EQ.0.0) GO TO 596
IF (XEND-XFLO.GE.XCLLS) GO TO 570
C.....DETERMINE IF THE OBSERVATION POINT SEES THE [NF].....
596 IF (XCONV.EQ.0.0) GO TO 597
IF (XEND-XFLO.GE.XCONV) GO TO 560
C.....THE OBSERVATION POINT SEES THE [VNF].....
597 GO TO 559
553 WRITE(3,746) STM
GO TO 417
C.....CALCULATE THE CONCENTRATION USING THE [VNF] MODEL FOR.....
C.....A STEADY FLOW RIVER AFTER THE CONTINUOUS SPILL HAS STOPPED.....
559 CONTINUE
GO TO 561
C.....CALCULATE THE CONCENTRATION USING THE [NF] MODEL FOR A.....
C.....STEADY FLOW RIVER AFTER THE CONTINUOUS SPILL HAS STOPPED.....
560 CONTINUE
561 LOC(1,1)=AI*OC
LOC(2,1)=WC-ALOC
LOC(3,1)=AI*OC
LOC(4,1)=-WC-ALOC
LOC(5,1)=AI*OC
LOC(1,2)=-Y(1,6)
LOC(2,2)=-Y(1,6)
LOC(3,2)=2.0*DC+Y(1,6)
LOC(4,2)=-Y(1,6)
LOC(5,2)=Y(1,6)
OMFOA=(UR*UR+4.0*KNF*EXNF)**0.5
CONCEN=0.0
DO 510 IJJ 1,5
RSUBN=((XOBS+XPS)**2.0+(EXNF/EYNF)*((Y0BS-LOC(IJJ,1)
1)**2.0)+(EXNF/EZNF)*((Z0BS-LOC(IJJ,2))**2.0))**0.5

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ERFN(1)=(RSUBN+OMEGA*(STM-SPTIME))/((4.0*EXNF*(STM-SPTIME))**0.5)
ERFN(2)=(RSUBN+OMEGA*STM)/((4.0*EXNF*STM)**0.5)
ERFN(3)=(RSUBN-OMEGA*(STM-SPTIME))/((4.0*EXNF*(STM-SPTIME))**0.5)
ERFN(4)=(RSUBN-OMEGA*STM)/((4.0*EXNF*STM)**0.5)
DO 511 IJJJ 1,4
IF (ERFN(IJJJ).GT.8.0.OR.ERFN(IJJJ).LT.-8.0) EP=0.0
IF (ERFN(IJJJ).GT.8.0.OR.ERFN(IJJJ).LT.-8.0) GO TO 593
EP=EXP(-(ERFN(IJJJ)*ERFN(IJJJ)))
593 IF (ERFN(IJJJ).LT.0.0) IAE=1
IF (ERFN(IJJJ).GE.0.0) IAE=0
IF (ERFN(IJJJ).LT.0.0) ERFN(IJJJ)=-ERFN(IJJJ)
ERFN(IJJJ)=1.0-(0.34802/(1.0+0.47047*ERFN(IJJJ))-0.09587/((1.0+0.4
17047*ERFN(IJJJ))**2.0)+0.74785/((1.0+0.47047*ERFN(IJJJ))*(1.0+
20.47047*ERFN(IJJJ))*(1.0+0.47047*ERFN(IJJJ)))*
3(EXP(-ERFN(IJJJ)**2.0))
511 IF (IAE.EQ.1) ERFN(IJJJ)=-ERFN(IJJJ)
ORPXU=(OMEGA*RSUBN+(X0BS+XPS)*UR)/(2.0*EXNF)
IF (ORPXU.GT.86.0.OR.ORPXU.LT.-86.0) ORPXU=0.0
IF (ORPXU.GT.86.0.OR.ORPXU.LT.-86.0) GO TO 510
ORPXU=EXP(ORPXU)
510 CONCEN=CONCEN+(1.0/RSUBN)*((ORPXU)*(ERFN(1)-ERFN(2))+EXP((-OMEGA
1*RSUBN+(X0BS+XPS)*UR)/(2.0*EXNF))*(ERFN(3)-ERFN(4)))
CONCEN=CONCEN*MASS/(25.1327*((EYNF*EZNF)**0.5))
GO TO 550
C.....CALCULATE THE CONCENTRATION USING THE [IF] MODEL FOR. .....
C.....A STEADY FLOW RIVER AFTER THE CONTINUOUS SPILL HAS STOPPED. .....
570 CONTINUE
OMEGAB=(UR*UR+4.0*KIF*EXIF)**0.5
SUMAT=0.0
CONCEN=0.0
DO 512 IKK=1,20
AKK=IKK
WSQ=(AKK**2.0)*9.8696*EYIF/(WC**2.0)
ERFI(1)=(STM*((OMEGAB**2.0+4.0*EXIF*WSQ)**0.5)+(X0BS+XLS))/
1((4.0*EXIF*STM)**0.5)
ERFI(2)=((STM-SPTIME)*((OMEGAB**2.0+4.0*EXIF*WSQ)**0.5)+
1(X0BS+XLS))/((4.0*EXIF*(STM-SPTIME))**0.5)
ERFI(3)=(STM*((OMEGAB**2.0+4.0*EXIF*WSQ)**0.5)-(X0BS+XLS))/
1((4.0*EXIF*STM)**0.5)
ERFI(4)=((STM-SPTIME)*((OMEGAB**2.0+4.0*EXIF*WSQ)**0.5)-
1(X0BS+XLS))/((4.0*EXIF*(STM-SPTIME))**0.5)
DO 513 IKKK=1,4
IF (ERFI(IKKK).GT.8.0.OR.ERFI(IKKK).LT.-8.0) EP=0.0
IF (ERFI(IKKK).GT.8.0.OR.ERFI(IKKK).LT.-8.0) GO TO 590
EP=EXP(-(ERFI(IKKK)*ERFI(IKKK)))
590 IF (ERFI(IKKK).LT.0.0) IAE=1
IF (ERFI(IKKK).GE.0.0) IAE=0
IF (ERFI(IKKK).LT.0.0) ERFI(IKKK)=-ERFI(IKKK)
ERFI(IKKK)=1.0-(0.34802/(1.0+0.47047*ERFI(IKKK))-0.09587/((1.0+0.4
17047*ERFI(IKKK))*(1.0+0.47047*ERFI(IKKK)))+0.74785/
2((1.0+0.47047*ERFI(IKKK))*(1.0+0.47047*ERFI(IKKK))*(1.0+0.47047*_
3ERFI(IKKK)))*EP
513 IF (IAE.EQ.1) ERFI(IKKK)=-ERFI(IKKK)
XSRPXU=(X0BS+XLS)*((OMEGAB**2.0+4.0*EXIF*WSQ)**0.5)/
1(2.0*EXIF)
IF (XSRPXU.GT.86.0.OR.XSRPXU.LT.-86.0) XSRPXU=0.0
IF (XSRPXU.GT.86.0.OR.XSRPXU.LT.-86.0) GO TO 512
XSRPXU=EXP(XSRPXU)
512 SUMAT=SUMAT+(((1.0+4.0*EXIF*KIF/(UR*UR))**0.5)*(COS(IKK*PI*_
1((WC/2.0)+AI*DC)/WC)*(COS(IKK*PI*((Y0BS+WC/2.0)/WC))))/
2(((1.0+4.0*EXIF*(KIF+WSQ)/(UR*UR))**0.5)*((XSRPXU)*(ERFI(1)-
3ERFI(2))+EXP((-X0BS+XLS)*((OMEGAB**2.0+4.0*EXIF*WSQ
4)**0.5)+(X0BS+XLS)*UR)/(2.0*EXIF))*(ERFI(3)-ERFI(4)))

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SUMAT=2. 0*SUMAT
ERFI(1)=((XOBS+XLS)+OMEGAB*STM)/((4. 0*EXIF*STM)**0. 5)
ERFI(2)=((XOBS+XLS)+OMEGAB*(STM-SPTIME))/((4. 0*EXIF*
1(STM-SPTIME))**0. 5)
ERFI(3)=((OMEGAB*STM-(XOBS+XLS))/((4. 0*EXIF*STM)**0. 5)
ERFI(4)=((OMEGAB*(STM-SPTIME)-(XOBS+XLS))/((4. 0*EXIF*
1(STM-SPTIME))**0. 5)
DO 514 IKKKK=1,4
IF (ERFI(IKLLL). GT. 8. 0. OR. ERF(IKLLL). LT. -8. 0) EP=0. 0
IF (ERFI(IKLLL). GT. 8. 0. OR. ERF(IKLLL). LT. -8. 0) GO TO 591
EP=EXP(-(ERFI(IKLLL)*ERFI(IKLLL)))
591 IF (ERFI(IKLLL). LT. 0. 0) IAE=1
IF (ERFI(IKLLL). GE. 0. 0) IAE=0
IF (ERFI(IKLLL). LT. 0. 0) ERF(IKLLL)=-ERFI(IKLLL)
ERFI(IKLLL)=1. 0-(0. 34802/(1. 0+0. 47047*ERFI(IKLLL))-0. 09587/((1. 0+
10. 47047*ERFI(IKLLL))*(1. 0+0. 47047*ERFI(IKLLL)))+0. 74785/
2((1. 0+0. 47047*ERFI(IKLLL))*(1. 0+0. 47047*ERFI(IKLLL))*
3(1. 0+0. 47047*ERFI(IKLLL)))*EP
514 IF (IAE. EQ. 1) ERF(IKLLL)=-ERFI(IKLLL)
OXXU=(OMEGAB*(XOBS+XLS)+(XOBS+XLS)*UR)/(2. 0*EXIF)
IF (OXXU. GT. 86. 0. OR. OXXU. LT. -86. 0) OXXU=0. 0
IF (OXXU. GT. 86. 0. OR. OXXU. LT. -86. 0) GO TO 519
OXXU=EXP(OXXU)
519 CONCEN=OXXU*(ERFI(1)-ERFI(2))+(EXP((-OMEGAB*(XOBS+XLS)
1+(XOBS+XLS)*UR)/(2. 0*EXIF)))*(ERFI(3)-ERFI(4))
CONCEN=CONCEN+SUMAT
CONCEN=CONCEN*(MASS/(2. 0*WC*DC*UR*((1. 0+4. 0*EXIF*KIF/(UR*UR))**0. 5
1)))
GO TO 550
C..... CALCULATE THE CONCENTRATION USING THE [FF] MODEL FOR A STEADY.
C..... FLOW RIVER AFTER THE CONTINUOUS SPILL HAS STOPPED. ....
C
580 TYPE *, 'FF'
OMEGB=(UR*UR+4. 0*KFF*EXFF)**0. 5
ERFF(1)=(OMEGB*STM+(XOBS+XFF))/((4. 0*EXFF*STM)**0. 5)
ERFF(2)=(OMEGB*(STM-SPTIME)+(XOBS+XFF))/((4. 0*EXFF*(STM-
1SPTIME))**0. 5)
ERFF(3)=(OMEGB*STM-(XOBS+XFF))/((4. 0*EXFF*STM)**0. 5)
ERFF(4)=(OMEGB*(STM-SPTIME)-(XOBS+XFF))/((4. 0*EXFF*(STM-
1SPTIME))**0. 5)
DO 515 ILL=1,4
IF (ERFF(ILL). GT. 8. 0. OR. ERF(ILL). LT. -8. 0) EP=0. 0
IF (ERFF(ILL). GT. 8. 0. OR. ERF(ILL). LT. -8. 0) GO TO 592
EP=EXP(-(ERFF(ILL)*ERFF(ILL)))
592 IF (ERFF(ILL). LT. 0. 0) IAE=1
IF (ERFF(ILL). GE. 0. 0) IAE=0
IF (ERFF(ILL). LT. 0. 0) ERF(ILL)=-ERFF(ILL)
ERFF(ILL)=1. 0-(0. 34802/(1. 0+0. 47047*ERFF(ILL))-0. 09587/((1. 0+0. 470
147*ERFF(ILL))*(1. 0+0. 47047*ERFF(ILL)))+0. 74785/
2((1. 0+0. 47047*ERFF(ILL))*(1. 0+0. 47047*ERFF(ILL))*
3(1. 0+0. 47047*ERFF(ILL)))*EP
515 IF (IAE. EQ. 1) ERF(ILL)=-ERFF(ILL)
XUPOBX=((XOBS+XFF)*OMEGB+(XOBS+XFF)*UR)/(2. 0*EXFF)
IF (XUPOBX. GT. 86. 0. OR. XUPOBX. LT. -86. 0) XUPOBX=0. 0
IF (XUPOBX. GT. 86. 0. OR. XUPOBX. LT. -86. 0) GO TO 518
XUPOBX=EXP(XUPOBX)
518 CONCEN=MASS/(2. 0*WC*DC*UR*((1. 0+4. 0*EXFF*KFF/(UR*UR))**0. 5))*
1(XUPOBX*(ERFF(1)-ERFF(2))+(EXP((-XOBS+XFF)*OMEGB+
2(XOBS+XFF)*UR)/(2. 0*EXFF)))*(ERFF(3)-ERFF(4)))
GO TO 550
C..... CHEMICAL MASS IS NO LONGER BEING ADDED TO THE PLUME AT THE. ...
C..... SPILL LOCATION. ....
500 WRITE(3, 740)

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XCLLSS=XCLLS-XPS
XXIFF=XXIF-XLS
XFF=XFS-XXIF+XLS
IF (XCONV. GE. XEND) XCONV=0.0
IF (XCONV. EQ. 0.0) XCLLSS=0.0
IF (XCLLSS GE. XEND) XCLLSS=0.0
IF (XCLLSS. EQ. 0.0) XXIFF=0.0
IF (XXIFF. GE. XEND) XXIFF=0.0
CO TO 351
998 WRITE(3,732)
  TYPE *, 'TURBULENCE FACTOR MULTIPLIED BY ALFA 3 IS ZERO.'
  TYPE *, 'RUN TERMINATED.'
  TYPE *, '
999 CONTINUE
C
C***** FORMATS FOR INPUT STATEMENTS*****
99 FORMAT(6X, I3)
600 FORMAT(2X, F9.3, 4X, F9.3, 8X, F9.3, 9X, F9.3)
601 FORMAT(4X, F9.3, 7X, F9.3, 4X, F5.1, 5X, F8.3)
602 FORMAT(7X, A8)
603 FORMAT(4A8)
604 FORMAT(7X, F7.1, 8X, E11.4, 9X, F10.1)
605 FORMAT(7X, F10.1, 9X, F10.1)
606 FORMAT(3X, F9.3, 5X, F9.3, 7X, F9.3, 7X, F9.3)
607 FORMAT(4X, F10.5, 6X, F10.5, 6X, F10.5)
608 FORMAT(7X, F10.5, 9X, F10.5, 9X, F6.3, 9X, F7.3)
609 FORMAT(3X, I2, 5X, I2, 5X, I2)
C
C***** FORMATS FOR OUTPUT STATEMENTS*****
702 FORMAT(//4X, 18HINITIAL CONDITIONS/)
703 FORMAT(//4X, 16HFINAL CONDITIONS/)
704 FORMAT(6X, 50HO INITIAL DOWNSTREAM DISTANCE TO FIRST PRINT
10UI = , F12.4, 2H M/6X, 54HO INCREMENTAL DOWNSTREAM DISTANCE
2 BETWEEN PRINTOUTS = , F12.4, 2H M)
705 FORMAT(6X, 27HO INITIAL PLUME FLOWRATE = , E11.4, 7H M**3/S
1/6X, 17HO TIDAL PERIOD = , F10.1, 8H SECONDS
2/6X, 24HO TOTAL TIME OF SPILL = , F10.1, 8H SECONDS
3/6X, 50HO TIME INCREMENT FOR CONCENTRATION CALCULATIONS = , F10.1,
48H SECONDS
5/6X, 38HO MAXIMUM TIME FOR SPILL EVALUATION = , F10.1, 8H SECONDS
6/6X, 21HO WIDTH OF CHANNEL = , F9.3, 2H M
7/6X, 21HO DEPTH OF CHANNEL = , F9.3, 2H M)
706 FORMAT(6X, 58HO DISTANCE FROM THE CHANNEL CENTERLINE TO THE SPILL
1 ORIGIN/8X, 21HIN THE Y DIRECTION = , F10.3, 2H M
2/6X, 55HO DISTANCE FROM THE CHANNEL SURFACE TO THE SPILL ORIGIN
3/8X, 21HIN THE Z DIRECTION = , F10.3, 2H M
4/6X, 44HO NEAR FIELD MODEL DECAY RATE COEFFICIENT = , F10.5
5/6X, 52HO INTERMEDIATE FIELD MODEL DECAY RATE COEFFICIENT = , F10.5
6/6X, 43HO FAR FIELD MODEL DECAY RATE COEFFICIENT = , F10.5
7/6X, 53HO LAMBDA COEFFICIENT FOR THE VERY NEAR FIELD MODEL = , F10.5
8)
707 FORMAT(6X, 69HO RATIO OF CIRCUMFERENTIAL TO CENTERLINE CONCENTRATION
1 FOR CONVERSION/8X, 26H10 THE NEAR FIELD MODEL = , F10.5
2/6X, 68HO ERROR BETWEEN THE NEAR FIELD AND INTERMEDIATE FIELD
3 CONCENTRATIONS/8X, 29HAT THE POINT OF CONVERSION = , F10.5
4/6X, 62HO DISTANCE INCREMENT FOR THE INTERMEDIATE FIELD MODEL
5 MATCHING/8X, 10HROUTINE = , F10.5, 2H M)
708 FORMAT(2X, 10HTEST NO. : , A8)
709 FORMAT(/2X, 24HFLOW FIELD DESCRIPTION: , 4A8/)
710 FORMAT(6X, 31HO CHANNEL REFERENCE VELOCITY = , F6.3, 4H M/S
1/6X, 18HO PLUME DENSITY = ,
2F10.3, 8H KG/M**3/6X, 32HO PLUME CHARACTERISTIC RADIUS = , F12.3, 2H

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3 M/6X, 44HO PLUME VELOCITY (STREAM SPEED COMPONENT) = , F12. 5, 4H M/S
 4/6X, 45HO PLUME ANGLE (WITH RESPECT TO HORIZONTAL) = , F12. 5, 8H RADI
 5ANS/6X, 45HO INITIAL X (HORIZONTAL DISTANCE FROM VENT) = , F12. 5, 2H
 6M/6X, 44HO INITIAL Z (VERTICAL DEPTH FROM SURFACE) = , F12. 5, 2H M//)

711 FORMAT(//5X, 38HVERY NEAR FIELD PLUME CENTERLINE PATH:
 1//7X, 1HX, 14X, 1HZ, 10X, 17HCONCENTRATION(CL)/4X, 8H(METERS), 7X,
 28H(METERS), 10X, 9H(KG/M**3)//)

712 FORMAT(6X, 31HO MEAN VELOCITY OF THE RIVER = , F10. 3, 4H M/S/
 1 6X, 31HO ORIENTATION OF THE SPILL JET:)

713 FORMAT(8X, 32HPLUME RADIUS FROM OOMS' MODEL = , F12. 4, 7H METERS
 1//9X, 1HY, 8X, 13HCONCENTRATION/5X, 8H(METERS), 7X, 9H(KG/M**3)//)

714 FORMAT(30H NUMERICAL INTEGRATION DATA//7X, 19HO STARTING POINT
 1=, F10. 4/7X, 22HO INITIAL STEP SIZE=, F10. 6/7X, 20HO FINAL
 2 STEP SIZE=, F10. 6//)

715 FORMAT(/2X, 21HJET DIRECTION CHANGED//)

716 FORMAT(/2X, F9. 3, 3X, E11. 4)

717 FORMAT(1H1, /2X, 12HSTEADY RIVER//)

718 FORMAT(//9X, 1HY, 8X, 13HCONCENTRATION/5X, 8H(METERS), 7X, 9H(KG/M**3)//)

719 FORMAT(28H ENTRAINMENT COEFFICIENTS//7X, 11HO ALFA 1=, F8. 4/7X,
 111HO ALFA 2=, F8. 4/7X, 11HO ALFA 3=, F8. 4//)

725 FORMAT(X, 27HALFA3 * TURBULENCE LEVEL = , F10. 5)

726 FORMAT(1H1)

727 FORMAT(2X, 33H1URBULENT DIFFUSION COEFFICIENTS: //7X,
 17HExNF = , E11. 4/7X, 7HEYNF = , E11. 4/7X, 7HEZNF = , E11. 4//7X,
 27HExIF = , E11. 4/7X, 7HEYIF = , E11. 4//7X, 7HEXFF = , E11. 4//)

728 FORMAT(1H1, //2X, 22HMODEL CONVERSION DATA://
 12X, 46HTHE CONVERSION FROM THE VERY NEAR FIELD TO THE/2X, 27HNEAR
 2 FIELD BEGINS AT XCL = , F10. 2, 2H M/2X, 69HTHE ADJUSTMENT IN THE X
 3 DIRECTION AT THE POINT OF CONVERSION FROM THE/2X, 42HVERY NEAR
 4 FIELD TO THE NEAR FIELD MODEL = , F12. 4, 2H M/2X, 60HTHE CENTERLINE
 5 CONCENRATION AT THE POINT OF CONVERSION FROM/2X, 40HTHE VERY NEAR
 6 FIELD TO THE NEAR FIELD = , E12. 4, 8H KG/M**3)

729 FORMAT(1H1, //2X, 22HMODEL CONVERSION DATA://
 12X, 56HTHE CONVERSION FROM THE [VNFM] BUOYANT PLUME MODEL TO THE/
 22X, 51H[VNF] GRAVITY SPREADING PLUME MODEL OCCUURS AT XCL=, F10. 2,
 22H M//.
 32X, 55HTHE DEPTH OF THE PLUME CENTER LINE BELOW THE SURFACE = ,
 3 F7. 2, 2H M//.
 42X, 58HTHE CENTERLINE CONCENTRATION AT THE CONVERSION POINT IS = ,
 4 E12. 4, 8H KG/M**3)

730 FORMAT(/2X, 60H1HE CONVERSION FROM THE [VNFM] GRAVITY SPREADING MODE
 1L TO THE/
 22X, 46H[IF] INTERMEDIATE FIELD MODEL OCCURS AT XCL = , F10. 2, 2H M//.
 32X, 46HTHE [IF] VERTICAL LINE SOURCE CONCENTRATION = , E11. 4,
 3 8H KG/M**3/
 42X, 55HTHE LOCATION OF THE VIRTUAL ORIGIN FOR THE [IF] MODEL = ,
 4 F10. 2, 2H M/
 42X, 32HUPSTREAM OF THE CONVERSION POINT/
 52X, 56HTHE RATIO OF THE INTERMEDIATE FIELD CONCENTRATION TO THE/
 52X, 49H[VNF] CONCENTRATION FOR THIS ORIGIN DISTANCE IS = , F10. 5//)

731 FORMAT(6X, 31HO CHANNEL REFERENCE VELOCITY = , F6. 3, 4H M/S
 1/6X, 35HO PLUME CENTERLINE CONCENTRATION = , F10. 3, 8H KG/M**3
 2/6X, 39HO PLUME CONSTANT CONCENTRATION WIDTH = , F10. 3, 2H M
 3/6X, 26HO PLUME EFFECTIVE WIDTH = , F10. 3, 2H M
 4/6X, 40HO PLUME CROSS STREAM DISPERSION LENGTH = , F10. 3, 2H M
 5/6X, 37HO PLUME VERTIAL DISPERSION LENGTH = , F10. 3, 2H M
 6/6X, 47HO FINAL X (HORIZONTAL DISTANCE FOR DISCHARGE)= , F10. 3, 2H M
 7/6X, 41HO FINAL Z (VERTICAL DEPTH FROM SURFACE)= , F10. 3, 2H M)

732 FORMAT(/2X, 63H1URBULENCE FACTOR MULTIPLIED BY ALFA 3 IS ZERO. RUN
 1 TERMINATED.)

733 FORMAT(/2X, 41H1HE CONVERSION FROM THE NEAR FIELD TO THE/2X, 35H
 1INTERMEDIATE FIELD BEGINS AT XCL = , F12. 4, 2H M
 2/2X, 39H1HE INTERMEDIATE FIELD CONCENTRATION = , E11. 4,

38H KG/M**3)
 734 FORMAT(2X, F12. 4, 3X, F12. 4, 7X, E11. 4)
 735 FORMAT(//4X, 47HTURBULENCE FACTORS FOR THE NEAR FIELD EQUATION: /
 1/7X, 21H0 EY COEFFICIENT = , F10. 5/7X, 21H0 EZ COEFFICIENT = , F10
 2. 5//)
 736 FORMAT(6X, 26H0 AMBIENT FLUID DENSITY = , F9. 3, 8H KG/M**3/6X, 33H0 DI
 1SPERSION JET FLUID DENSITY = , F9. 3, 8H KG/M**3/6X, 24H0 AMBIENT TEMP
 2ERATURE = , F5. 1, 12H DEG RANKINE/
 36X, 27H0 INITIAL PLUME DIAMETER = , F9. 4, 3H CM/6X,
 42H0 CHANNEL TURBULENCE LEVEL = , F5. 3)
 737 FORMAT(2X, 60HTHE ADJUSTMENT IN THE X DIRECTION AT THE POINT OF
 1 CONVERSION/2X, 54HFROM THE NEAR FIELD TO THE INTERMEDIATE FIELD
 2 MODEL = , F12. 4, 2H M/2X, 67HTHE RATIO OF THE INTERMEDIATE FIELD
 3 CONCENTRATION TO THE NEAR FIELD/2X, 39HCONCENTRATION FOR THE X
 4 OFFSET VALUE = , F10. 5//)
 738 FORMAT(1H1, 6X, 38HCONCENTRATION AT THE OBSERVATION POINT//
 18X, 47HDOWNSTREAM DISTANCE TO THE OBSERVATION POINT = , F12. 3, 2H M
 2/8X, 61HDISTANCE FROM THE CHANNEL SURFACE TO THE OBSERVATION
 3 LOCATION/8X, 21HIN THE Z DIRECTION = , F10. 3, 2H M/8X,
 45H (THE Z VALUE IS THE SPILL CENTERLINE LOCATION)
 5/8X, 19H0BSERVATION TIME = , F10. 1, 8H SECONDS
 6/8X, 34HTRANSVERSE INCREMENTAL DISTANCE = , F12. 3, 7H METERS)
 739 FORMAT(1H1, 6X, 38HCONCENTRATION AT THE OBSERVATION POINT//
 18X, 47HDOWNSTREAM DISTANCE TO THE OBSERVATION POINT = , F12. 3, 2H M
 2/8X, 61HDISTANCE FROM THE CHANNEL SURFACE TO THE OBSERVATION
 3 LOCATION/8X, 21HIN THE Z DIRECTION = , F10. 3, 2H M
 4/8X, 19H0BSERVATION TIME = , F10. 1, 8H SECONDS
 5/8X, 34HTRANSVERSE INCREMENTAL DISTANCE = , F12. 3, 7H METERS)
 740 FORMAT(/6X, 25HTHE SPILL HAS TERMINATED. //)
 744 FORMAT(4X, F10. 3, 5X, E11. 4//)
 746 FORMAT(/2X, 7HTIME = , F10. 1, 5X, 50HTHE ENTIRE PLUME HAS PASSED
 1 THE OBSERVATION POINT. //)
 747 FORMAT(2X, 49HTHE CONVERSION FROM THE INTERMEDIATE FIELD TO THE
 1/2X, 26HFAIR FIELD BEGINS AT XCL = , F12. 4, 2H M
 2/2X, 60HTHE ADJUSTMENT IN THE X DIRECTION AT THE POINT OF
 3 CONVERSION/2X, 53HFROM THE INTERMEDIATE FIELD TO THE FAIR FIELD
 4 MODEL = , F12. 4, 2H M)
 751 FORMAT(6X, 26H HORIZONTAL DOWNSTREAM)
 752 FORMAT(6X, 24H HORIZONTAL UPSTREAM)
 753 FORMAT(6X, 20H VERTICAL UPWARD)
 754 FORMAT(6X, 22H VERTICAL DOWNWARD)
 755 FORMAT(6X, 39H HORIZONTAL TRANSVERSE TO THE RIGHT)
 756 FORMAT(6X, 38H HORIZONTAL TRANSVERSE TO THE LEFT)
 780 FORMAT(/5X, 50HSWITCH TO VERY NEAR FIELD GRAVITY SPREADING MODEL)
 781 FORMAT(/55H X CA SY SZ B BEFF
 1. /58H (METERS) (KG/M**3) (METERS) (METERS) (METERS) (METERS))
 787 FORMAT(1H1)
 788 FORMAT(F8. 2, E12. 4, F8. 3, F9. 3, F9. 3, F9. 3)
 END

C

 C
 SUBROUTINE RHS2(Y, RS)
 DIMENSION Y(3), RS(3)
 COMMON/PHYS/DCOR, EPS, UPRI, ROA, DENS, G, UR, UA
 COMMON/HCS1/C1, C2, C3, C4, C5, C6, DPLU
 COMMON/HQS2/AFM1, AFM12, DELRO, CA, Z0, B2M1, CAI
 C LIST OF VARIABLES
 C Y(1) = (SZ/Z0)**AF1
 C Y(2) = BEFF
 C Y(3) = SY**2
 C
 SZ = Z0*(Y(1)**AFM1)

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      ROCA = ROA + DELRO*CA
C*** DIFFERENTIAL EQUATION FOR BEFF
      IF (DENS.GT.ROA) RS(2)=C5*SQRT(1.-ROA/ROCA)*((SZ/Z0)**AFM12)
      IF (DENS.LT.ROA) RS(2)=C5*SQRT(1.-ROCA/ROA)*((SZ/Z0)**0.5)
C
C*** DIFFERENTIAL EQUATION FOR SY**2
C
      RS(3) = C6*(Y(2)**B2M1)
C
C*** DIFFERENTIAL EQUATION FOR (SZ/Z0)**AF1
C
C      COMPUTE RICHARDSON NUMBER
C
      HFFF = C7*SZ
      RICH = C3*HFFF
      APHI = 0.62 + 1.3911*(RICH**0.7)
C
      RS(1) = C1/APHI - Y(1)*RS(2)/Y(2)
C
      RETURN
      END
```

```

C *****PROGRAM OOMS*****
C
C PROJECT NO. : 02-5864-003
C PROJECT SPONSOR: COAST GUARD
C DATE: 5-27-81
C
C THIS PROGRAM PREDICTS PLUME TRAJECTORY AND PLUME CONCENTRATION
C OF A BUOYANT PLUME USING OOMS' METHOD.
C
C INPUT DATA FILES: SPILLIN.DAT
C OUTPUT DATA FILES: SPILLOUT.DAT
C
C INTEGER FUNCTION HAMING( N, Y, F, X, H, TE)
C
C FUNCTION HAMING IS TAKEN FROM 'APPLIED NUMERICAL METHODS' BY
C B. CARNahan, H. A. LUTHER, AND J. O. WILKES, PUBLISHED BY J. WILEY
C AND SONS, INC. 1969. PAGES 401 TO 402.
C
C HAMING IMPLEMENTS HAMMING'S PREDICTOR-CORRECTOR ALGORITHM TO
C SOLVE N SIMULTANEOUS FIRST-ORDER ORDINARY DIFFERENTIAL
C EQUATIONS. X IS THE INDEPENDENT VARIABLE AND H IS THE
C INTEGRATION STEPSIZE. THE ROUTINE MUST BE CALLED TWICE FOR
C INTEGRATION ACROSS EACH STEP. ON THE FIRST CALL, IT IS ASSUMED
C THAT THE SOLUTION VALUES AND DERIVATIVE VALUES FOR THE N
C EQUATIONS ARE STORED IN THE FIRST N COLUMNS OF THE FIRST
C FOUR ROWS OF THE Y MATRIX AND THE FIRST THREE ROWS OF THE F
C MATRIX, RESPECTIVELY. THE ROUTINE COMPUTES THE N PREDICTED
C SOLUTIONS YPRED(J), INCREMENTS X BY H AND PUSHES ALL
C VALUES IN THE Y AND F MATRICES DOWN ONE ROW. THE PREDICTED
C SOLUTIONS YPRED(J) ARE MODIFIED, USING THE TRUNCATION ERROR
C ESTIMATES TE(J) FROM THE PREVIOUS STEP, AND SAVED IN THE FIRST
C ROW OF THE Y MATRIX. HAMING RETURNS TO THE CALLING PROGRAM WITH
C THE VALUE 1 TO INDICATE THAT ALL DERIVATIVES SHOULD BE COMPUTED
C AND STORED IN THE FIRST ROW OF THE F ARRAY BEFORE THE SECOND
C CALL IS MADE ON HAMING. ON THE SECOND ENTRY TO THE FUNCTION
C (DETERMINED BY THE LOGICAL VARIABLE PRED), HAMING USES THE
C HAMMING CORRECTOR TO COMPUTE NEW SOLUTION ESTIMATES, ESTIMATES
C THE TRUNCATION ERRORS TE(J) FOR THE CURRENT STEP, IMPROVES
C THE CORRECTED SOLUTIONS USING THE NEW TRUNCATION ERROR
C ESTIMATES, SAVES THE IMPROVED SOLUTIONS IN THE FIRST ROW OF THE
C Y MATRIX, AND RETURNS TO THE CALLING PROGRAM WITH A VALUE 2 TO
C INDICATE COMPLETION OF ONE FULL INTEGRATION STEP.
C
C LOGICAL PRED
C DIMENSION YPRED(20), TE(N), Y(4,N), F(3,N)
C DATA PRED / .TRUE. /
C
C ..... IS CALL FOR PREDICTOR OR CORRECTOR SECTION .....
C IF (.NOT. PRED) GO TO 4
C
C ..... PREDICTOR SECTION OF HAMING .....
C ..... COMPUTE PREDICTED Y(J) VALUES AT NEXT POINT .....
C DO 1 J=1,N
1 YPRED(J) = Y(4,J) + 4.*H*(2.*F(1,J) - F(2,J) + 2.*F(3,J))/3.
C
C ..... UPDATE THE Y AND F TABLES .....
C DO 2 J=1,N
C DO 2 K5=1,3
K = 5 - K5
Y(K,J) = Y(K-1,J)
2 IF (K.LT.4) F(K,J) = F(K-1,J)
C

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```

C      .... MODIFY PREDICTED Y(J) VALUES USING THE TRUNCATION ERROR
C      .... ESTIMATES FROM THE PREVIOUS STEP. INCREMENT X VALUE
C      DO 3 J=1,N
3      Y(1,J) = YPRED(J) + 112.*TE(J)/9.
      X = X + H
C
C      .... SET PRED AND REQUEST UPDATED DERIVATIVE VALUES .....
PRED = .FALSE.
HAMING = 1
RETURN
C
C      .... CORRECTOR SECTION OF HAMING
C      .... COMPUTE CORRECTED AND IMPROVED VALUES OF THE Y(J) AND SAVE
C      .... TRUNCATION ERROR ESTIMATES FOR THE CURRENT STEP .....
4      DO 5 J=1,N
      Y(1,J) = (9.*Y(2,J)-Y(4,J) + 3.*H*(F(1,J)+2.*F(2,J)-F(3,J)))/8.
      TE(J) = 9.*(Y(1,J) - YPRED(J))/121.
5      Y(1,J) = Y(1,J) - TE(J)
C
C      .... SET PRED AND RETURN WITH SOLUTIONS FOR CURRENT STEP .....
PRED = .TRUE.
HAMING = 2
RETURN
END
INTEGER FUNCTION RUNGE(N, Y, F, X, H)
C
C      FUNCTION RUNGE IS TAKEN FROM 'APPLIED NUMERICAL METHODS' BY
C      B. CARNAHAN, H. A. LUTHER, AND J. O. WILKES, PUBLISHED BY J. WILEY
C      AND SONS, INC. 1969. PAGES 374 TO 375.
C
C      THE FUNCTION RUNGE EMPLOYS THE FOURTH-ORDER RUNGE-KUTTA METHOD
C      WITH KUTTA'S COEFFICIENTS TO INTEGRATE A SYSTEM OF N SIMULTAN-
C      EOUS FIRST ORDER ORDINARY DIFFERENTIAL EQUATIONS F(J)=DY(J)/DX,
C      (J=1,2,...,N), ACROSS ONE STEP OF LENGTH H IN THE INDEPENDENT
C      VARIABLE X, SUBJECT TO INITIAL CONDITIONS Y(J), (J=1,2,...,N).
C      EACH F(J), THE DERIVATIVE OF Y(J), MUST BE COMPUTED FOUR TIMES
C      PER INTEGRATION STEP BY THE CALLING PROGRAM. THE FUNCTION MUST
C      BE CALLED FIVE TIMES PER STEP (PASS(1)...PASS(5)) SO THAT THE
C      INDEPENDENT VARIABLE VALUE (X) AND THE SOLUTION VALUES
C      (Y(1)...Y(N)) CAN BE UPDATED USING THE RUNGE-KUTTA ALGORITHM.
C      M IS THE PASS COUNTER. RUNGE RETURNS AS ITS VALUE 1 TO
C      SIGNAL THAT ALL DERIVATIVES (THE F(J)) BE EVALUATED OR 0 TO
C      SIGNAL THAT THE INTEGRATION PROCESS FOR THE CURRENT STEP IS
C      FINISHED. SAVEY(J) IS USED TO SAVE THE INITIAL VALUE OF Y(J)
C      AND PHI(J) IS THE INCREMENT FUNCTION FOR THE J(TH) EQUATION.
C      AS WRITTEN, N MAY BE NO LARGER THAN 50.
C
C      DIMENSION PHI(50), SAVEY(50), Y(N), F(N)
C      DATA M/0/
C
      M = M + 1
      GO TO (1,2,3,4,5), M
C
C      .... PASS 1 .....
1      RUNGE = 1
      RETURN
C
C      .... PASS 2 .....
2      DO 22 J=1,N
      SAVEY(J) = Y(J)
      PHI(J) = F(J)
22      Y(J) = SAVEY(J) + 0.5*H*F(J)
      X = X + 0.5*H

```

```

RUNGE = 1
RETURN

C
C ..... PASS 3 .....
3 DO 33 J= 1,N
PHI(J) = PHI(J) + 2.0*F(J)
33 Y(J) = SAVEY(J) + 0.5*H*F(J)
RUNGE = 1
RETURN

C
C ..... PASS 4 .....
4 DO 44 J= 1,N
PHI(J) = PHI(J) + 2.0*F(J)
44 Y(J) = SAVEY(J) + H*F(J)
X = X + 0.5*H
RUNGE = 1
RETURN

C
C ..... PASS 5 .....
5 DO 55 J = 1,N
55 Y(J) = SAVEY(J) + (PHI(J) + F(J))*H/6.0
M = 0
RUNGE = 0
RETURN
END

REAL FUNCTION SIMUL(N, A, X, EPS, INOIC, NRC)

C
C FUNCTION SIMUL IS TAKEN FROM 'APPLIED NUMERICAL METHODS' BY
C B. CARNahan, H. A. LUTHER, AND J. O. WILKES, PUBLISHED BY J. WILEY
C AND SONS, INC. 1969. PAGES 290 TO 291.

C
C WHEN INOIC IS NEGATIVE, SIMUL COMPUTES THE INVERSE OF THE N BY
C N MATRIX A IN PLACE. WHEN INOIC IS ZERO, SIMUL COMPUTES THE
C N SOLUTIONS X(1)...X(N) CORRESPONDING TO THE SET OF LINEAR
C EQUATIONS WITH AUGMENTED MATRIX OF COEFFICIENTS IN THE N BY
C N+1 ARRAY A AND IN ADDITION COMPUTES THE INVERSE OF THE
C COEFFICIENT MATRIX IN PLACE AS ABOVE. IF INOIC IS POSITIVE,
C THE SET OF LINEAR EQUATIONS IS SOLVED BUT THE INVERSE IS NOT
C COMPUTED IN PLACE. THE GAUSS-JORDAN COMPLETE ELIMINATION METHOD
C IS EMPLOYED WITH THE MAXIMUM PIVOT STRATEGY. ROW AND COLUMN
C SUBSCRIPTS OF SUCCESSIVE PIVOT ELEMENTS ARE SAVED IN ORDER IN
C THE IROW AND JCOL ARRAYS RESPECTIVELY. K IS THE PIVOT COUNTER,
C PIVOT THE ALGEBRAIC VALUE OF THE PIVOT ELEMENT, MAX
C THE NUMBER OF COLUMNS IN A AND DETERMINE THE DETERMINANT OF THE
C COEFFICIENT MATRIX. THE SOLUTIONS ARE COMPUTED IN THE (N+1) TH
C COLUMN OF A AND THEN UNSCRAMBLED AND PUT IN PROPER ORDER IN
C X(1)...X(N) USING THE PIVOT SUBSCRIPT INFORMATION AVAILABLE
C IN THE IROW AND JCOL ARRAYS. THE SIGN OF THE DETERMINANT IS
C ADJUSTED, IF NECESSARY, BY DETERMINING IF AN ODD OR EVEN NUMBER
C OF PAIRWISE INTERCHANGES IS REQUIRED TO PUT THE ELEMENTS OF THE
C JORD ARRAY IN ASCENDING SEQUENCE WHERE JORD(IROW(I)) = JCOL(I).
C IF THE INVERSE IS REQUIRED, IT IS UNSCRAMBLED IN PLACE USING
C Y(1)...Y(N) AS TEMPORARY STORAGE. THE VALUE OF THE DETERMINANT
C IS RETURNED AS THE VALUE OF THE FUNCTION. SHOULD THE POTENTIAL
C PIVOT OF LARGEST MAGNITUDE BE SMALLER IN MAGNITUDE THAN EPS,
C THE MATRIX IS CONSIDERED TO BE SINGULAR AND A TRUE ZERO IS
C RETURNED AS THE VALUE OF THE FUNCTION.

C
C DIMENSION IROW(15), JCOL(15), JORD(15), Y(15), A(NRC,NRC), X(N)

C
C MAX=N
C IF (INDIC.GE.0) MAX=N+1
C ... BEGIN ELIMINATION PROCEDURE...

```

```

DETER=1
DO 18 K=1,N
KM1=K-1
C   ... SEARCH FOR THE PIVOT ELEMENT...
PIVOT=0.
DO 11 I=1,N
DO 11 J=1,N
C   ... SCAN IROW AND JCOL ARRAYS FOR INVALID PIVOT SUBSCRIPTS...
IF (K.EQ.1) GO TO 9
DO 8 ISCAN=1,KM1
DO 8 JSCAN=1,KM1
IF (I.EQ.IROW(ISCAN)) GO TO 11
IF (J.EQ.JCOL(JSCAN)) GO TO 11
8 CONTINUE
9 IF (ABS(A(I,J)).LE.ABS(PIVOT)) GO TO 11
PIVOT=A(I,J)
IROW(K)=I
JCOL(K)=J
11 CONTINUE
C   ... INSURE THAT SELECTED PIVOT IS LARGER THAN EPS...
IF (ABS(PIVOT).GT.EPS) GO TO 13
WRITE(3,202)
SIMUL=0.
RETURN
C   ... UPDATE THE DETERMINANT VALUE...
13 IROWK=IROW(K)
JCOLK=JCOL(K)
DETER=DETER*PIVOT
C   ... NORMALIZE PIVOT ROW ELEMENTS...
DO 14 J=1,MAX
14 A(IROWK,J)=A(IROWK,J)/PIVOT
C   ... CARRY OUT ELIMINATION AND DEVELOP INVERSE...
A(IROWK,JCOLK)=1./PIVOT
DO 18 I=1,N
AIJCK=A(I,JCOLK)
IF (I.EQ.IROWK) GO TO 18
A(I,JCOLK) = -AIJCK/PIVOT
DO 17 J=1,MAX
17 IF (J.NE.JCOLK) A(I,J)=A(I,J)-AIJCK*A(IROWK,J)
18 CONTINUE
C   ... ORDER SOLUTION VALUES (IF ANY) AND CREATE JORD ARRAY...
DO 20 I=1,N
IROWI=IROW(I)
JCOLI=JCOL(I)
JORD(IROWI)=JCOLI
20 IF (INDIC.QE.0) X(JCOLI)=A(IROWI,MAX)
C   ... ADJUST SIGN OF DETERMINANT...
IN1CH=0
NM1=N-1
DO 22 I=1,NM1
IP1=I+1
DO 22 J=IP1,N
IF (JORD(J).QE.JORD(I)) GO TO 22
JTEMP=JORD(J)
JORD(J)=JORD(I)
JORD(I)=JTEMP
IN1CH=INTCH+1
22 CONTINUE
IF (INTCH/2*2.NE.INTCH) DETER=-DETER
C   ... IF INDIC IS POSITIVE RETURN WITH RESULTS...
IF (INDIC.LF.0) GO TO 26
SIMUL=DETER
RETURN

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```

C     ... IF INDIC IS NEGATIVE OR ZERO, UNSCRAMBLE THE INVERSE
C     FIRST BY ROWS...
26 DO 28 J=1,N
DO 27 I=1,N
IROWI=IROW(I)
JCOLI=JCOL(I)
27 Y(JCOLI)=A(IROWI,J)
DO 28 I=1,N
28 A(I,J)=Y(I)
C     ... THEN BY COLUMNS...
DO 30 I=1,N
DO 29 J=1,N
IROWJ=IROW(J)
JCOLJ=JCOL(J)
29 Y(IROWJ)=A(I,JCOLJ)
DO 30 J=1,N
30 A(I,J)=Y(J)
C     ... RETURN FOR INDIC NEGATIVE OR ZERO...
SIMUL=DETER
RETURN
202 FORMAT(37H03MAIL PIVOT - MATRIX MAY BE SINGULAR)
ENI)
SUBROUTINE RHS(Y,C)
DIMENSION Y(6),A(3,3),B(4,4),C(4),D(3)
COMMON/PHYS/DCDR,EPS,UPRI,ROA,DENS,Q,UR,UA
COMMON/CON2/ROT,ALFA1,ALFA2,ALFA3
C
C     VERY NEAR FIELD EQUATIONS FOR GAUSSIAN PROFILES AND VARIABLE DEN-
C     SITY.
C
ST= SIN(Y(4))
ST2=ST*ST
CT= COS(Y(4))
CT2=CT*CT
UA2=UA*UA
UACT=UA*CT
UAST=UA*ST
Y12=Y(1)*Y(2)
Y33=Y(3)*Y(3)
ROC=Y(1)/DCDR
ROCA=ROC/ROA
AC1=0.7/2699*UACT+0.412442*Y(3)
AC2=(1.043144*UACT + 0.55679*Y(3))/ROA
AC3=(1.043144*UACT*UACT + 1.113593*UACT*Y(3) + 0.363346*Y33)/ROA
AM1=2.*UACT*UACT + 1.729329*UACT*Y(3) + 0.490842*Y33
AMP=Y(2)*(1.729329*UACT+0.981684*Y(3)+ROCA*(1.113593*UACT
1    +0.726692*Y(3)))
C
C     CONSERVATION OF SPECIES
C
A(1,1)=Y(2)*AC1
A(1,2)=2.*Y(1)*AC1
A(1,3)=0.412442*Y12
A(1,4)=-0.772699*Y12*UAST
A(1,5)=0.
C
C     CONSERVATION OF MASS
C
A(2,1)=Y(2)*AC2/DCDR
A(2,2)=2.*((2.*UACT + 0.864665*Y(3) + ROC*AC2)
A(2,3)=Y(2)*((0.864665 + 0.556796*ROCA)
A(2,4)=Y(2)*UAST*(-2. -1.043144*ROCA)
A(2,5)=2.*((ALFA1* ABS(Y(3)) + ALFA2* UACT* ABS(ST) + ALFA3* UPRI)

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C
C      CONSERVATION OF X-MOMENTUM
C
A(3, 1)=Y(2)*AC3*CT/DCDR
A(3, 2)=2. *(AM1 + AC3*ROC)*CT
A(3, 3)=CT*AM2
A(3, 4)=Y(2)*ST*(-6. *UACT*UACT-3. 458658*UACT*Y(3)-0. 490842*Y33
1 -ROCA*(3. 129432*UACT*UACT+2. 227186*UACT*Y(3)+0. 363346*Y33))
A(3, 5)=UA*A(2, 5)+0. 3*UAP* ABS(ST*ST*ST)

C
C      CONSERVATION OF Y-MOMENTUM
C
A(4, 1)=Y(2)*ST*AC3/DCDR
A(4, 2)=2. *ST*(AM1 + AC3*ROC)
A(4, 3)=ST*AM2
A(4, 4)=Y(2)*(2. *UA2*CT*(1. -3. *ST2)+1. 729329*UA*Y(3)*(CT2-ST2)
1 +0. 490842*Y33*CT + ROCA*(1. 043144*UA2*CT*(1. -3. *ST2)
2 +1. 113593*Y(3)*UA*(CT2-ST2) + 0. 363346*Y33*CT))
IF (ST. LT. 0. ) GO TO 40
SIC=-1.
GO TO 45
40 SIC=1.
45 CONTINUE
A(4, 5)=-1. 043144*ROCA*Y(2)*G + SIG*0. 3*UAST*UAST*CT

C
C      SIMUL USED FOR MATRIX INVERSION
C
DETER=SIMUL(4, A, C, EPS, 1, 5)
RETURN
END

```

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DTIC